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ACTA PHYSICA POLONICA

DWUMIESIĘCZNIK

Vol. XVII — Fasc. 1

WARSZAWA 1958

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PAŃSTWOWE WYDAWNICTWO NAUKOWE

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CONTENTS

FASCICULUS 1

Leruste Ph., Représentation legrangienne d'un fluide parfait	3
Rubinowicz A., Ein bisher nicht beachteter Fall, in dem der Kirchhoffsche Ansatz zur angenäherten Beschreibung der Beugungserscheinungen versagt	13
Sawicki J. and Szymański Z., Nucleon-Surface Interaction and the (p,n) Reactions	21
Wardzyński W., Investigation of Infrared Absorption in Alkali Halide Crystals with Anionic Impurities	29
Galasiewicz Z., The Problem of the Subsidiary Conditions in the Additional Variables Method for Arbitrary Central Interactions	63
Hryniewicz A. Z., Waluga T. and Zapalski G., An Experiment on Nonadiabatic Passage in Nuclear Magnetic Resonance	71
Reviews of Books	77

FASCICULUS 2—3

Halaubrenner J., On the Influence of the Anisotropy of the Base on the Resistance of a Rolling Cylinder	83
Auleytner J. and Kołakowski B., Microscopic Observations on the Surface of InSb Monocrystals	93
Ostrowski K. and Turek L., Radiation Accompanying Pulses in a Geiger—Müller Counter	97
Auleytner J., Determination of the Orientation of Mosaic Blocks by Means of a Fine-Focus X-Ray Tube	111
Łopuszański J., On the Modification of the Feynman's "Integral-Over-All-Paths" Method	117
Rayski J., On a Possible Relation Between Space and Iso-Space	137
Białynicki-Birula I., On the Internal Degress of Freedom of Particle in Quantum Field Theory	153
Barashenkov V. S., and Maltsev V. M., Multiple Product on of Nonstable Particles in Pion Nucleon Collisions	177
Sharma H. D., Threshold Potential for the Low Frequency Electric Discharge in Air Using a Maze Counter	183
Rayski J., An Attempt to Geometrize Mesoelectrodynamics	187

Letters to the Editor

Gołębiowski A. and Zalewski K., On the Interpretation of Slater's Approximation of Atomic Orbitals	199
Kołos W., On the Electron Density Distribution in Molecules	201

Laboratory Equipment and Techniques

Benisz J. and Borowczak C., A New Method for the Rapid Measurement for the Shrinkage Factor of a Nuclear Emulsion . . .	203
---	-----

FASCICULUS 4

Piekara A. and Kielich S., A Non-Linear Theory of the Electric Permittivity and Refractivity of Dielectric Liquids in Electric and Magnetic Fields	209
Kielich S., Semi-Macroscopic Treatment of the Theory of Non-Linear Phenomena in Dielectric Liquids Submitted to Strong Electric and Magnetic Fields	239
Wojciechowski K. F., Thermoemission of Alloys	257
Kopeć Z., Investigation of the Effective Mass of Current Carriers in GaSb	265
O'Connor D., A Simplified Method of Solution for a Random Walk Problem of a Few Unequal Steps	273

FASCICULUS 5

Kociński J., On the Influence of the Demagnetizing Field of Domain Structure	283
Kusch W., Measurement of Absorption in Graphite of Electrons from Meson μ Decay	295
Mościcki W., On the Use of G.M. Counters Filled with a Mixture of $\text{CO}_2 + \text{CS}_2$ for the Measurement of the Activity of Natural Carbon. Part I.	311
Mościcki W., On the Use of G.M. Counters Filled with a Mixture of $\text{CO}_2 + \text{CS}_2$ for the Measurement of the Activity of Natural Carbon. Part II.	327
Liszk a L. and Niewodniczański H., Intensity Ratio in the "Forbidden" Doublet λ 2958 and λ 2972 Å.U. in the Spectrum of Atomic Oxygen	345
Hryniewicz A. Z., The Application of Magnetic Nuclear Resonance in Fluid Hydrodynamics	353

Laboratory Equipment and Techniques

Kisiel A. and Niewodniczański H., A High Luminosity Quartz Spectograph of the far Ultra-Violet Region λ 2300—1850 Å.U.	361
--	-----

Letters to the Editor

Leś Z. and Niewodniczański H., Intensity Ratios of Spectral Lines in Cd I Triplets at Different Conditions of Excitation . . .	365
--	-----

FASCICULUS 6

Miąsek M., The Application of the Tight Binding Method to the Investigation of Energy Bands in Hexagonal Close-Packed Structure. III.	371
---	-----

Bartenbach M., Buras B., Rzewuski H. and Tomczak Z., Steady Stimulation and Quenching of Photoconductivity in Cadmium Sulfide by Infrared Radiation	389
Barashenkov V. S. and Maltsev V. M., On the Magnitude of Strange Particle Production Cross-Section in Nucleon-Nucleon Collisions at Cosmotron Energy	397
Massalski J. M. and Oleś A., On the Ratio of Photons to Electrons in Extensive Air Showers of Cosmic Radiation Found from Analysis of the Transition Curve	401
Babecki J., Analysis of the Influence of Low-Energy Penetrating Photons on the Absorption of Extensive Air Showers in Lead	409
Rzewuski J., The 13-Parametric Group of Transformation of the Spinor Space and its Representations	417
Minardi E., On the Bilocal Theory of the Electron	429
Morkowski J., Reversible Susceptibility Under Stress	435
Kunisz M. D., Rapports des intensités des raies spectrales dans certains doublets des séries II et I secondaires des spectres d'arc d'aluminium et d'indium	455
Śledzik J., Bohm and Pines Collective Description of Electron Interactions in Crystals. Part I.	463
Jabłoński A., Corrections and Additional Remarks to the Paper: Self Depolarization and Decay of Photoluminescence of Solutions, Acta phys. Polon., 14, 295 (1955)	481

Letters to the Editor

Janik J. A., Kraśnicki S. and Murasik A., The Influence of Polarization of Liquid Crystals Molecules on the Scattering of Slow Neutrons	483
Janik J. A., Mańiawski F. and Rżany H., Teoretical Calculation of the Slow Neutron Scattering Cross Section of Ethylene-Molecule	489

Reviews of Books

Weyssenhoff J., Wilhelm Macke	491
---	-----

AUTHOR INDEX

Auleytner J. and Kołakowski B., Microscopic Observations on the Surface of InSb Monocrystals	93
Auleytner J., Determination of the Orientation of Mosaic Blocks by Means of a Fine-Focus X-Ray Tube	111
Babecki J., Analysis of the Influence of Low-Energy Penetrating Photons on the Absorption of Extensive Air Showers in Lead	409
Barashenkov V. S., and Maltsev V. M., Multiple Production of Nonstable Particles in Pion Nucleon Collisions	177
Barashenkov V. S. and Maltsev V. M., On the Magnitude of Strange Particle Production Cross-Section in Nucleon-Nucleon Collisions at Cosmotron Energy	397

Bartenbach M., Buras B., Rzewuski H. and Tomczak Z., Steady Stimulation and Quenching of Photoconductivity in Cadmium Sulfide by Infrared Radiation	389
Benisz J. and Borowczak C., A New Method for the Rapid Measurement for the Shrinkage Factor of a Nuclear Emulsion	203
Białyński-Birula I., On the Internal Degree of Freedom of Particle in Quantum Field Theory	153
Galasiewicz Z., The Problem of the Subsidiary Conditions in the Additional Variables Method for Arbitrary Central Interactions	63
Gołębiowski A. and Zalewski K., On the Interpretation of Slater's Approximation of Atomic Orbitals	199
Halaunbrenner J., On the Influence of the Anisotropy of the Base in the Resistance of a Rolling Cylinder	83
Hryniewicz A. Z., Waluga T. and Zapalski G., An Experiment of Nonadiabatic Passage in Nuclear Magnetic Resonance	71
Hryniewicz A. Z., The Application of Magnetic Nuclear Resonance in Fluid Hydrodynamics	353
Jabłoński A., Corrections and Additional Remarks to the Paper: Self Depolarization and Decay of Photoluminescence of Solutions, <i>Acta phys. Polon.</i> , 14 , 295 (1955)	481
Janik J. A., Kraśnicki S. and Murasik A., The Influence of Polarization of Liquid Crystals Molecules on the Scattering of Slow Neutrons	483
Janik J. A., Maniawski F. and Rżany H., Teoretical Calculation of the Slow Neutron Scattering Cross Section of Ethylene-Molecule	489
Kielich S., Semi-Macroscopic Treatment of the Theory of Non-Linear Phenomena in Dielectric Liquids Submitted to Strong Electric and Magnetic Fields	239
Kisiel A. and Niewodniczański H., A High Luminosity Quartz Spectograph of the far Ultra-Violet Region λ 2300—1850 Å.U.	361
Kociński J., On the Influence of the Demagnetizing Field of Domain Structure	283
Kołos W., On the Electron Density Distribution in Molecules	201
Kopeć Z., Investigation of the Effective Mass of Current Carriers in GaSb	265
Kunisz M. D., Rapports des intensités des raies spectrales dans certains doublets des séries II et I secondaires des spectres d'arc d'aluminium et d'indium	455
Kusch W., Measurement of Absorption in Graphite of Electrons from Meson μ Decay	295
Leruste Ph., Représentation lagrangienne d'un fluide parfait	3
Leś Z. and Niewodniczański H., Intensity Ratios of Spectral Lines in Cd I Triplets at Different Conditions of Excitation	365
Liszka L. and Niewodniczański H., Intensity Ratio in the "Forbidden" Doublet λ 2958 and λ 2972 Å.U. in the Spectrum of Atomic Oxygen	345

Lopuszański J., On the Modification of the Feynman's "Integral-Over-All-Paths" Method	117
Massalski J. M. and Oleś A., On the Ratio of Photons to Electrons in Extensive Air Showers of Cosmic Radiation Found from Analysis of the Transition Curve	401
Miąsek M., The Application of the Tight Binding Method to the Investigation of Energy Bands in Hexagonal Close-Packed Structure. III.	371
Minardi E., On the Bilocal Theory of the Electron	429
Morkowski J., Reversible Susceptibility Under Stress	435
Mościcki W., On the Use of G.M. Counters Filled with a Mixture of $\text{CO}_2 + \text{CS}_2$ for the Measurement of the Activity of Natural Carbon. Part I.	311
Mościcki W., On the Use of G.M. Counters Filled with a Mixture of $\text{CO}_2 + \text{CS}_2$ for the Measurement of the Activity of Natural Carbon. Part II.	327
O'Connor D., A Simplified Method of Solution for a Random Walk Problem of a Few Unequal Steps	273
Ostrowski K. and Turek L., Radiation Accompanying Pulses in a Geiger-Müller Counter	97
Piekara A. and Kielich S., A Non-Linear Theory of the Electric Permittivity and Refractivity of Dielectric Liquids in Electric and Magnetic Fields	209
Rayski J., On a Possible Relation Between Space and Iso-Space	137
Rayski J., An Attempt to Geometrize Mesoelectrodynamics	187
Rubinowicz A., Ein bisher nicht beachteter Fall, in dem der Kirchhoffsche Ansatz zur angenäherten Beschreibung der Beugungerscheinungen versagt	13
Rzewuski J., The 13-Parametric Group of Transformations of the Spinor Space and its Representations	417
Sawicki J. and Szymański Z., Nucleon-Surface Interaction and the (p,n) Reactions	21
Sharma H. D., Threshold Potential for the Low Frequency Electric Discharge in Air Using a Maze Counter	183
Śledzik J., Bohm and Pines Collective Description of Electron Interactions in Crystals. Part. I.	463
Wardzyński W., Investigation of Infrared Absorption in Alkali Halide Crystals with Anionic Impurities	29
Weyssenhoff J., Wilhelm Macke	491
Wojciechowski K. F., Thermoemission of Alloys :	257

REPRESENTATION LAGRANGIENNE D'UN FLUIDE PARFAIT

PAR PHILIPPE LERUSTE

*(Manuscrit reçu le 3 octobre 1957)**I. Lagrangiens d'un milieu homogène isotrope*

Ordinairement en mécanique des champs (Pauli 1941, sans quantification) on exprime qu'un champ possède l'invariance de Lorentz par la condition nécessaire et suffisante que sa fonction de Lagrange \mathcal{L} soit un scalaire, c'est à dire un tenseur d'ordre zéro de l'espace-temps. Cette fonction de Lagrange est fonction du (ou des) champ ψ , de $\partial_\mu \psi$ et aussi des quantités $C^{(i)}(x)$ qui sont des tenseurs qui définissent le milieu dans lequel le (ou les) champ se propage (comme exemple courant, ces quantités sont les composantes d'un champ électromagnétique extérieur). Les quantités \mathcal{L} et $C^{(i)}(x)$ ont des grandeurs tensorielles quelconques.

Admettons qu'un développement de \mathcal{L} en série entière soit possible, on peut alors écrire:

$$\mathcal{L} = \sum_n a_n P_n(\psi, \partial_\mu \psi, C^{(i)}(x)) \quad (1.1)$$

où P_n est un polynôme homogène de degré n par rapport à l'ensemble des variables et où a_n sont des nombres. \mathcal{L} se présente alors sous forme d'une somme et pour que \mathcal{L} soit un scalaire il faut et il suffit que P_n soit un produit contracté d'ordre zéro. Or de tels produits peuvent s'exprimer à partir d'un nombre fini d'entre eux, dont le choix est d'ailleurs arbitraire et que nous appellerons scalaires fondamentaux formés avec ψ , $\partial_\mu \psi$ et $C^{(i)}(x)$. En définitive \mathcal{L} apparaît comme une fonction des scalaires fondamentaux formés avec ψ , $\partial_\mu \psi$ et $C_{(i)}(x)$.

Si le milieu où s'effectue la propagation de ψ est homogène cela impose aux quantités $C^{(i)}(x)$ d'être des quantités indépendantes de x , d'où:

$$C^{(i)}(x) = C^{(i)} \quad (1.2)$$

Si le milieu est isotrope cela impose aux quantités $C^{(i)}(x)$ de n'admettre autour du point x aucune direction privilégiée. Ces quantités ne peuvent donc représenter un vecteur, ni un tenseur d'ordre supérieur ni, de même, un spineur (auquel sont attachés des éléments tensoriels de l'espace-temps). Les $C^{(i)}(x)$ ne peuvent donc être que des scalaires (ou pseudoscalaires).

Si le milieu est à la fois homogène et isotrope, il est donc défini par des scalaires indépendants de x , c'est à dire par des nombres. On peut alors faire rentrer ces nombres dans les coefficients de \mathcal{L} et on peut énoncer alors:

Dans un milieu homogène et isotrope, \mathcal{L} est une fonction des scalaires fondamentaux formés avec ψ , $\partial_\mu \psi$ et $C^{(i)}(x)$.

II. Cas de deux champs scalaires réels

Soient R et S deux champs scalaires réels¹. Dans \mathcal{L} interviennent aussi $\partial_\mu R$ et $\partial_\mu S$. Nous prendrons comme système de scalaires fondamentaux:

$$\begin{cases} X_1 = R, \\ X_2 = \frac{1}{2} \partial_\mu R \partial^\mu R, \\ X_3 = \frac{1}{2} \partial_\mu S \partial^\mu S, \\ X_4 = \partial_\mu R \partial^\mu S, \\ X_5 = S. \end{cases} \quad (2.1)$$

Tous les autres scalaires que l'on peut former sont fonction de ceux-ci. En particulier le carré du bivecteur défini par $\partial_\mu R$ et $\partial_\mu S$ s'évalue par une identité de Lagrange:

$$\begin{aligned} (\partial_\mu R \partial_\nu S - \partial_\nu R \partial_\mu S)^2 &= (\partial_\rho R \partial^\rho R) (\partial_\sigma S \partial^\sigma S) - (\partial_\lambda R \partial^\lambda S)^2, \\ (\partial_\mu R \partial_\nu S - \partial_\nu R \partial_\mu S)^2 &= 4 X_2 X_3 - X_4^2. \end{aligned} \quad (2.2)$$

D'après ce qui a été vu au paragraphe précédent la fonction de Lagrange de deux tels champs se propageant dans un milieu homogène-isotrope est:

$$\mathcal{L} = L(X_1, X_2, X_3, X_4, X_5). \quad (2.3)$$

Nous poserons:

$$\begin{cases} L_1 = \frac{\partial L}{\partial X_1}, \\ L_2 = \frac{\partial L}{\partial X_2}, \\ \dots \dots \dots \\ L_3 = \frac{\partial L}{\partial X_3}, \end{cases} \quad (2.4)$$

Avec ces notations les équations de champ s'écrivent:

$$\partial^\mu (L_2 \partial_\mu R + L_4 \partial_\mu S) = L_1, \quad (2.5)$$

$$\partial^\mu (L_3 \partial_\mu S + L_4 \partial_\mu R) = L_1. \quad (2.6)$$

¹ Il est facile de passer de ce cas, au cas d'un seul champ imaginaire en posant $\psi = R \exp iS$. Inversement l'équation de Klein-Gordon se ramène à une fonction de Lagrange de ce type.

Nous serons amenés à utiliser un courant:

$$j_\mu = \frac{\partial \mathcal{L}}{\partial (\partial_\mu S)} = L_3 \partial_\mu S + L_4 \partial_\mu R, \quad (2.7)$$

pour que celui-ci soit conservatif il faut et il suffit que:

$$L_5 \equiv 0. \quad (2.8)$$

Avec cette condition:

$$\partial^\mu j_\mu = 0 \quad (2.9)$$

Que (2.8) soit vérifiée ou non, le tenseur énergie-impulsion s'écrit:

$$T_{\mu\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_\mu R)} \partial_\nu R + \frac{\partial \mathcal{L}}{\partial (\partial_\mu S)} \partial_\nu S - \mathcal{L} g_{\mu\nu},$$

$$T_{\mu\nu} = L_2 \partial_\mu R \partial_\nu R + L_3 \partial_\mu S \partial_\nu S + L_4 (\partial_\mu S \partial_\nu R + \partial_\mu R \partial_\nu S) - L g_{\mu\nu}. \quad (2.10)$$

D'après la mécanique des champs:

$$\partial^\nu T_{\mu\nu} = 0 \quad (2.11)$$

relation qui peut être vérifiée directement.

Le tenseur moment cinétique interne est nul, le tenseur énergie-impulsion canonique étant symétrique.

III. Fluide relativiste

Pour un fluide relativiste on admet que le courant est vecteur propre du tenseur énergie-impulsion du genre temps (Synge 1937, Lichnerowicz 1955). Pour que le formalisme du paragraphe 2 soit apte à représenter un tel fluide il est nécessaire que le courant j_μ soit vecteur propre de $T_{\mu\nu}$, c'est à dire que l'on ait:

$$T_{\mu\nu} j^\nu = -\varrho j_\mu \quad (3.1)$$

ϱ étant la densité du fluide au sens de la mécanique relativiste². Selon (2.7) et (2.10) on peut évaluer le premier membre. Posant:

$$k_\mu = L_3 \partial_\mu S - L_4 \partial_\mu R,$$

$$2 L_3 L_4 T_{\mu\nu} = j_\mu [(L_2 L_3 + L_4^2) \partial_\nu R + 2 L_2 L_3 \partial_\nu S] -$$

$$- 2 L_3 L_4 L g_{\mu\nu} + k_\mu [(L_4^2 - L_2 L_3) \partial_\nu R], \quad (3.2)$$

² Le signe — provient de la signature + + + — qui est utilisée. Les calculs sont menés dans l'espace de la relativité restreinte. Aucune raison de principe ne semble empêcher l'extension à la relativité générale.

$$2 L_3 L_4 T_{\mu\nu} j^\nu = j_\mu \{ (L_2 L_3 + L_4^2) (j^\nu \partial_\nu R) + 2 (L_3 L_4) (j^\nu \partial_\nu S + 2 L_3 L_4) \} + k_\mu [(L_4^2 - L_2 L_3) j^\nu \partial_\nu R]. \quad (3.3)$$

Cette quantité est proportionnelle à j_μ si, et seulement si, l'une des deux relations suivantes est vérifiée, avec l'aide de (2.1) et (2.7):

$$j^\nu \partial_\nu R \equiv L_3 X_4 + 2 L_4 X_2 = 0, \quad (3.4)$$

$$L_4^2 - L_2 L_3 = 0. \quad (3.5)$$

Nous supposons que nous nous trouvons dans un cas non dégénéré et que L_2 , L_3 et L_4 ne sont pas identiquement nuls.

a) Cas où $L_3 X_4 + 2 X_4 X_2 = 0$.

On voit facilement dans l'équation (3.3) que la valeur propre $-\varrho$ est:

$$-\varrho = j^\nu \partial_\nu R - L = 2 L_3 X_3 + L_4 X_4 - L. \quad (3.6)$$

On voit de même que $\partial_\mu R$ est un vecteur propre de $T_{\mu\nu}$ avec pour valeur propre p_1 :

$$2 L_3 L_4 p_1 = (k_\mu \partial^\mu R) (L_4^2 - L_2 L_3) - 2 L_2 L_4 L$$

compte tenu de (3.4):

$$p_1 = -2 X_2 \frac{L_4^2 - L_2 L_3}{L_3} - L. \quad (3.7)$$

Tout vecteur A_μ perpendiculaire aux deux précédents, c'est à dire tel que, $A_\mu j^\mu = 0$, $A_\mu \partial^\mu R = 0$, donc aussi $A_\mu k^\mu = 0$, est vecteur propre avec pour valeur propre:

$$p_2 = p_3 = -L. \quad (3.8)$$

Dans ce cas si le formalisme lagrangien est apte à représenter un fluide relativiste, ce fluide est nécessairement particulier puisque l'ellipsoïde des tensions possède selon (3.8) deux axes égaux. Pour avoir le fluide le plus général il aurait fallu partir d'une fonction de Lagrange de 3 champs R , S et T .

Toutefois nous ne considérerons que le cas d'un fluide parfait où:

$$p_1 = p_2 = p_3 = p.$$

Cette condition impose selon (3.7) et (3.8), si l'on écarte la solution dégénérée $X_2 \equiv 0$:

$$L_4^2 - L_2 L_3 = 0,$$

c'est la solution (3 - 5) déjà rencontrée. L'examen du cas a) ramène donc automatiquement pour le problème posé au cas b).

b) Cas où $L_4^2 - L_2 L_3 = 0$.

En ce cas on peut mettre $T_{\mu\nu}$ sous la forme:

$$T_{\mu\nu} = \frac{j_\mu j_\nu}{L_3} - L g_{\mu\nu} = \frac{D^2}{L_3} u_\mu u_\nu - L g_{\mu\nu}, \quad (3.9)$$

la densité ϱ est donnée par:

$$-\varrho = -\frac{D^2}{L_3} - L \quad (3.10)$$

en posant:

$$-D^2 = j_\mu j^\mu = 2(L_3^2 X_3 + L_4^2 X_2 + L_3 L_4 X_4), \quad (3.11)$$

la pression est:

$$p = p_1 = p_2 = p_3 = -L \quad (3.12)$$

IV. Identification avec le fluide de Synge

Les notations nouvelles dans cette partie conformes à celles utilisées par Synge (1937). Dans son article Synge définit un courant A_μ dont le module est la fonction indice F ; mais ce courant n'est pas conservatif, c'est à dire que: $\partial^\mu A_\mu$ n'est pas identiquement nul:

$$\partial^\mu A_\mu \neq 0 \quad (4.1)$$

Par contre si on pose:

$$j_\mu = \frac{\varrho + p}{F} u_\mu = \frac{\varrho + p}{F^2} A_\mu \quad (4.2)$$

(u_μ est un vecteur unitaire porté par j_μ et A_μ) alors d'après les relations données par Synge (équations (9.2) et (9.3) par exemple) on a:

$$\partial^\mu j_\mu = 0. \quad (4.3)$$

Nous identifions ce vecteur j_μ déduit de la théorie de Synge au vecteur j_μ précédent tiré de la mécanique des champs. Soit:

$$j_\mu = D u_\mu = \frac{\varrho + p}{F} u_\mu,$$

d'où:

$$D = \frac{\varrho + p}{F}. \quad (4.4)$$

Identifions de même les tenseurs énergie-impulsion des deux théories.

$$T_{\mu\nu} = \frac{D^2}{L_3} u_\mu u_\nu - L g_{\mu\nu} = (\varrho + p) u_\mu u_\nu + p g_{\mu\nu},$$

d'où:

$$\frac{D^2}{L_3} = q + p, \quad (4.5)$$

$$p = -L, \quad (4.6)$$

ce qui est la correspondance (3.10), (3.12).

Cette correspondance est nécessaire. Nous verrons au paragraphe 6 qu'elle n'entraîne pas de contradiction.

De (4.4) et (4.5):

$$F = \frac{D}{L_3}, \quad (4.7)$$

d'où:

$$A_\mu = \frac{D}{L_3} u_\mu = \frac{j_\mu}{L_3},$$

de: (2.7)

$$A_\mu = \partial_\mu S + A \partial_\mu R \quad (4.8)$$

en posant pour simplifier:

$$A = \frac{L_4}{L_3} \quad (4.9)$$

V. Condition relative au rotationnel

Synge introduit un tenseur tourbillon dynamique:

$$\Omega_{\mu\nu} = \frac{1}{2} (\partial_\mu A_\nu - \partial_\nu A_\mu). \quad (5.1)$$

A l'aide de la formule (4.8) ce tenseur tourbillon peut s'écrire:

$$\Omega_{\mu\nu} = \frac{1}{2} (\partial_\mu A \partial_\nu R - \partial_\nu A \partial_\mu R) \quad (5.2)$$

L'une des conditions de Synge (équation (10.8)) est que $\Omega_{\mu\nu} A^\nu = 0$ ou, ce qui revient au même:

$$\Omega_{\mu\nu} j^\nu = 0 \quad (5.3)$$

cette relation s'écrit:

$$\partial_\mu A (j^\nu \partial_\nu R) - \partial_\mu R (j^\nu \partial_\nu A) = 0 \quad (5.4)$$

Les vecteurs $\partial_\mu A$ et $\partial_\mu R$ ne sont pas identiquement parallèles sinon le tenseur tourbillon serait identiquement nul ce que nous ne supposons pas. Donc, pour que l'équation précédente soit vérifiée, il faut et il suffit que:

$$j^\nu \partial_\nu R \equiv L_3 X_4 + 2 L_4 X_2 = 0 \quad (3.4)$$

$$j^\nu \partial_\nu A = 0. \quad (5.5)$$

La première équation avait été trouvée au paragraphe 3 mais on avait alors à imposer soit la condition (3.4) soit la condition (3.5). La suite du développement montre donc qu'on a à imposer ces deux relations simultanément et en outre la condition (5.5).

Intégrons d'abord le système (3.4) (3.5). Ce système équivaut au système:

$$L_4 X_4 + 2 L_2 X_2 = 0, \quad (5.6)$$

$$L_3 X_4 + 2 L_4 X_2 = 0. \quad (3.4)$$

Ce système aux dérivées partielles linéaire est intégrable ce qui montre que les conditions précédentes ne sont pas incompatibles avec la forme de L choisie à priori. Son intégrale générale se met sous la forme (M étant une fonction de deux variables):

$$L = M(\varphi_1, \varphi_2) \quad (5.7)$$

avec:

$$\begin{aligned} \varphi_1 &= X_1 \\ \varphi_2 &= \frac{4 X_2 X_3 - X_4^2}{4 X_2} \end{aligned} \quad (5.8)$$

on a pour les dérivées partielles:

$$\begin{aligned} L_1 &= M_1, \\ L_2 &= \frac{1}{4} M_2 \frac{X_4^2}{X_2^2}, \\ L_3 &= M_2, \\ L_4 &= -\frac{1}{2} M_2 \frac{X_4}{X_2}, \\ L_5 &= 0. \end{aligned} \quad (5.9)$$

En particulier le terme précédemment introduit:

$$A = \frac{L_4}{L_3} = -\frac{1}{2} \frac{X_4}{X_2}. \quad (5.10)$$

On voit facilement que les équations de champ peuvent s'écrire:

$$\partial^\mu [M_2 A (\partial_\mu S + A \partial_\mu R)] = M_1, \quad (5.11)$$

$$\partial^\mu [M_2 (\partial_\mu S + A \partial_\mu R)] \equiv \partial^\mu j_\mu = 0. \quad (5.12)$$

L'équation (5.11) s'écrit, compte tenu de (5.12):

$$\partial^\mu A \cdot [M_2 (\partial_\mu S + A \partial_\mu R)] = M,$$

soit :

$$\partial^\mu A \cdot j_\mu = M_1$$

Donc pour que la relation (5.5) soit satisfaite il faut et il suffit que :

$$M_1 (\equiv L_1) \equiv 0. \quad (5.13)$$

En définitive nous avons pu montrer que si une fonction de Lagrange $L(X_1, X_2, X_3, X_4, X_5)$ représente un fluide parfait, nécessairement cette fonction est de la forme (φ étant une fonction d'une seule variable) :

$$\begin{aligned} \mathcal{L} &= \varphi \left(\frac{4 X_2 X_3 - X_4^2}{4 X_2} \right) \\ &= \varphi \left((\partial_\mu S \partial^\mu S) - \frac{(\partial_\sigma R \partial^\sigma S)^2}{2(\partial_\sigma R \partial^\sigma R)} \right). \end{aligned} \quad (5.14)$$

On peut remarquer qu'interviennent dans \mathcal{L} le carré du produit extérieur de $\partial_\mu R$ et $\partial_\mu S$, d'après la formule (2.2) et le carré de $\partial_\mu R$.

VI. Réciproque

Nous allons montrer réciproquement qu'étant donné une fonction de Lagrange de la forme (5.14) on peut définir les quantités hydrodynamiques de la théorie de Synge-Lichnerowicz et que ces quantités obéissent aux égalités données par Synge par exemple. Nous ne chercherons pas à définir le cas où cette solution est unique. Nous ne chercherons pas non plus à restreindre L pour que les quantités ρ (densité) ou p (pression) soient définies positives, c'est à dire que nous ne cherchons pas les inégalités de la théorie classique.

Soit :

$$\mathcal{L} = \varphi \left(X_3 - \frac{X_4^2}{4 X_2} \right) \quad (5.14)$$

où X_2, X_3, X_4 sont définis par (2.1).

Soit φ' la dérivée de φ , la théorie des champs permet d'écrire :

$$j_\mu = \varphi \cdot (\partial_\mu S + A \partial_\mu R), \quad (6.1)$$

$$\partial^\mu j_\mu = 0, \quad (6.2)$$

$$D^2 = -j_\mu j^\mu = -2 \varphi'^2 \left(X_3 - \frac{X_4^2}{4 X_2} \right), \quad (6.3)$$

$$T_{\mu\nu} = \frac{D^2}{\varphi'} u_\mu u_\nu - \varphi g_{\mu\nu}, \quad (6.4)$$

$$\partial^\nu T_{\mu\nu} = 0. \quad (6.5)$$

Nous définirons les grandeurs de l'hydrodynamique classique en fonction des grandeurs de la mécanique des champs de la façon suivante, imposée par les relations précédentes:

— F par $D = \varphi' F$ qui est l'équation (4.7) car $L_3 \equiv \varphi'$, soit, selon (6.3):

$$-\frac{1}{2} F^2 = -\frac{1}{2} \frac{D^2}{\varphi'^2} = X_3 - \frac{X_4^2}{4 X_2} = \partial_\mu S \partial^\mu S - \frac{(\partial_e R \partial^e S)^2}{2(\partial_\sigma R \partial^\sigma R)} \quad (6.6)$$

— p par (équation (4.6)):

$$p = -\varphi \left(-\frac{1}{2} F^2\right) \quad (6.7)$$

— $\varrho(p)$ comme fonction implicite définie par l'équation qui sert ordinairement de définition à la fonction indice:

$$F = \exp \int_{p_0}^p \frac{dp}{\varrho(p) + p} \quad (6.8)$$

— la fonction $\mathcal{L} = \varphi$ qui est la fonction de Lagrange est définie en fonction de $\varrho(p)$ par l'ensemble de ces relations. Par élimination on peut encore la définir comme fonction implicite définie par la relation:

$$p = -\varphi \left(-\frac{1}{2} \exp 2 \int_{p_0}^p \frac{dp}{\varrho(p) + p} \right),$$

d'où une formule donnant sa fonction inverse φ^{-1} : $\varphi^{-1}[\varphi(X) = X]$

$$\varphi^{-1}(-X) = -\frac{1}{2} \exp 2 \int_{p_0}^X \frac{dp}{\varrho(p) + p'} \quad (6.9)$$

différenciant (6.7) et (6.8):

$$dF = F \frac{dp}{\varrho + p}$$

$$dp = \varphi' F dF$$

on tire;

$$\varphi' F^2 = \varrho + p, \quad (6.10)$$

en revombinant (6.6) et (6.10):

$$\frac{D^2}{\varphi'} = \varrho + p. \quad (6.11)$$

A l'aide de (6.7) et (6.11) on peut écrire le tenseur énergie-impulsion (6.4) sous la forme:

$$T_{\mu\nu} = (\varrho + p) u_\mu u_\nu + p g_{\mu\nu}. \quad (6.12)$$

Toutes les équations de Synge sont tirées des équations (6.5), (6.8), (6.12) (qui sont des conséquences de la théorie lagrangienne et de l'identification (6.6) à (6.8)), les autres équations de Synge sont donc aussi vérifiées.

Nous avons montré dans les paragraphes 3, 4, 5, que le formalisme lagrangien représentait le fluide parfait si on procédait à une identification rapplée de (6.6) à (6.8) et si \mathcal{L} avait une certaine forme (5.14). Dans le paragraphe 6 nous venons de montrer réciproquement qu' étant donné de cette forme et l'identification (6.6) à (6.8) alors les équations de Synge sont vérifiées. On a donc pu trouver une formulation lagrangienne pour le fluide parfait relativiste. Cette formulation a mis en évidence:

1) la différence entre la densité de la mécanique des champs D et celle de la relativité ϱ . On a trouvé entre elles la relation:

$$D = \frac{\varrho + P}{F} = \frac{r}{F} \quad (4.4)$$

r étant la pseudo-densité de M. Lichnérowicz.

2) A_μ n'est pas un courant, par contre, le tenseur énergie-impulsion s'écrivant:

$$T_{\mu\nu} = A_\mu j_\nu + p g_{\mu\nu} \quad (6.13)$$

A_μ peut être défini comme le vecteur énergie cinétique de l'unité de matière ayant la quadrivitesse u_μ .

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EIN BISHER NICHT BEACHTETER FALL, IN DEM DER KIRCHHOFFSCHE ANSATZ ZUR ANGENÄHERTEN BESCHREIBUNG DER BEUGUNGSERSCH EINUNGEN VERSAGT

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(Eingegangen am 17 September, 1957)

Es werden auf Grund eines Unabhängigkeitssatzes für die Kirchhoffsche Beugungswelle die Grenzen der Anwendbarkeit der durch den Kirchhoffschen Ansatz gegebenen Wellenbewegung zur Beschreibung der Beugungserscheinungen untersucht. Es zeigt sich dass dieser Ansatz nicht nur, wie bekannt, für sehr kleine oder sehr enge Beugungsöffnungen versagt, sondern auch unbrauchbar wird, falls der beugende Rand einen solchen Verlauf hat, dass es von der Lichtquelle ausgehende Halbgerade gibt, die durch zwei auf verschiedenen Teilen des beugenden Randes liegende Punkte genau oder angenähert hindurchgehen. Es werden die Konsequenzen besprochen, die sich aus diesem Versagen für die Gestalt der in der Kirchhoffschen Beugungstheorie verwendeten Schirme ergeben.

Im folgenden soll zunächst auf einen bisher, soweit mir bekannt ist, übersehenen Fall des Versagens des Kirchhoffschen Ansatzes zur angenäherten Beschreibung der Beugungserscheinungen hingewiesen werden. Sodann sollen die sich daraus für die Anwendung des Kirchhoffschen Ansatzes ergebenden Konsequenzen besprochen werden.

§ 1. Unabhängigkeitstheorem und Grenzen der Anwendbarkeit des Kirchhoffschen Ansatzes.

Für das folgende genügt es anzunehmen, daß wir es mit einem flächenhaften Schirm S zu tun haben, der eine einzige, ganz im Endlichen liegende Beugungsöffnung besitzt und sich sonst nach allen Seiten hin ins Unendliche erstreckt. Die durch den ursprünglichen Kirchhoffschen Ansatz gegebene Wellenfunktion u_K kann sodann in zwei Wellenbewegungen u_E und u_B aufgespalten¹ (S. 92 ff.) werden:

$$u_K = u_E + u_B. \quad (1.1)$$

¹ Bezüglich der Literaturangaben sei auf meine Monographie „Die Beugungswelle in der Kirchhoffschen Theorie der Beugung“ (Warszawa, 1957, Państwowe Wydawnictwo Naukowe) verwiesen. Die im folgenden in Klammern angegebenen Seitenzahlen beziehen sich auf diese Monographie.

u_E stellt die direkt einfallende Lichtwelle dar. Sie wird in allen Raumpunkten, in denen Licht gemäß der geometrischen Optik vorhanden ist, durch die Funktion $\exp(ikR)/R$ gegeben, die die unbehinderte Wellenausbreitung beschreibt. Außerhalb dieses Gebietes, d. h. im Schattenraume verschwindet jedoch u_E . R ist hier die Entfernung des Beobachtungspunktes P von der Lichtquelle L .

Die Funktion u_B wird als die Beugungswelle bezeichnet. Sie beschreibt eine Wellenbewegung, die ganz im Sinne der Youngschen Anschauungen durch die Streuung des direkt einfallenden Lichtes an den einzelnen Randelementen des beugenden Randes B entsteht. Sie wird durch das über B erstreckte Linienintegral

$$u_B = -\frac{1}{4\pi} \int_B \frac{e^{ik\varrho}}{\varrho} \frac{e^{ikr}}{r} \frac{\mathbf{r}(\varrho \times d\mathbf{s})}{r\varrho + r\varrho} \quad (1.2)$$

gegeben. Hier bedeutet ϱ bzw. r den von der Lichtquelle L bzw. dem Beobachtungspunkt P nach einem Bogenelement $d\mathbf{s}$ des beugenden Randes sich erstreckenden Vektor.

Wichtig ist für uns die Tatsache, daß die an einem bestimmten Randelement $d\mathbf{s}$ durch Streuung entstehende Wellenbewegung nur von der relativen Lage der Lichtquelle L und des betreffenden Randelementes $d\mathbf{s}$ abhängt. Von dem sonstigen Verlauf des beugenden Randes B ist jedoch diese Streuung vollkommen unabhängig. Um für diesen, für die Kirchhoffsche Beugungstheorie sehr charakteristischen Tatbestand eine kurze Bezeichnung zu haben, habe ich vor kurzem (S. 105) vorgeschlagen, ihn als das *Unabhängigkeitstheorem für die Beugungswelle* zu bezeichnen.

Dieses Theorem hat insbesondere zur Folge, daß in der Beugungswelle (1.2) keine Wellenbewegung enthalten ist, deren Entstehung durch eine nochmalige Streuung am beugenden Rande des hier bereits einmal gestreuten, direkt einfallenden Lichtes zu deuten wäre. Dem gegenüber kann man wohl nicht zweifeln, daß eine solche mehrfache Streuung bei den Wellenbewegungen, die im Falle von Beugungserscheinungen auftreten, tatsächlich zu erwarten ist. Man kann sich dies klar machen, falls man den Aufbau des stationären Zustandes einer solchen Wellenbewegung aus einem Anfangszustand heraus verfolgt, bei dem die einfallende Lichtwelle noch keinen der beugenden Körper erreicht hat (vgl. S. 283 ff.). Eine Nichtberücksichtigung dieser Wechselwirkung muß daher eine Beschränkung der Anwendbarkeit der durch den Kirchhoffschen Ansatz gegebenen Wellenbewegung u_K zur Approximation der bei der Beugung tatsächlich eintretenden Wellenvorgänge zur Folge haben.

In der Tat kann man auf diese Weise das bekannte Versagen des Kirchhoffschen Ansatzes für sehr kleine oder sehr enge Beugungsöffnungen verstehen. Mit Rücksicht auf den im Integranden der Beugungswelle (1.2) auftretenden Faktor $\exp(ikr)/r$, wächst nämlich die Amplitude der Beugungswelle mit der Annäherung an den beugenden Rand und wird mit abnehmender Entfernung vom beugenden Rande immer mehr vergleichbar mit der Amplitude des direkt einfallenden Lichtes, so daß eine wiederholte Streuung am beugenden Rande nicht mehr vernachlässigt werden kann.

Das gleiche Argument ist aber auch noch in einem anderen Falle anwendbar, der bisher der Aufmerksamkeit der Physiker entgangen zu sein scheint. Da die Wellenbewegung u_K , mit Ausnahme der Lichtquelle L , überall im Raume stetig ist, muß die Unstetigkeit der einfallenden Lichtwelle u_E in der Schattengrenze durch eine entsprechende hier auftretende Unstetigkeit der Beugungswelle u_B kompensiert werden. Daraus folgt, daß die Amplitude der Beugungswelle in der Schattengrenze mindestens von der gleichen Größenordnung sein muß, wie die der einfallenden Lichtwelle u_E . Dies ist tatsächlich der Fall (vgl. S. 194), wenn auch diese Amplitude mit wachsender Entfernung von der Schattengrenze rasch abnimmt.

Nehmen wir nun an, daß der beugende Rand eine solche Gestalt hat, daß ein Randelement ds ganz in der Nähe oder auch genau in der Schattengrenze eines anderen Bogenelementes ds' des beugenden Randes liegt. Auch in diesem Falle läßt sich selbstverständlich die durch den Kirchhoffschen Ansatz gegebene Wellenbewegung gemäß (1.1) ganz exakt in eine direkt einfallende und eine durch (1.2) gegebene Beugungswelle darstellen. Verwendet man also auch in diesem Falle den Kirchhoffschen Ansatz zur Beschreibung der Wellenbewegung, so berücksichtigt man nur die Streuung der direkt einfallenden Lichtwelle an dem Randelemente ds , nicht aber zugleich die Streuung der Beugungswelle des Randelementes ds' , die eine Amplitude von der gleichen Größenordnung hat. Der Kirchhoffsche Ansatz muß daher vor allem in jenen Raumpunkten versagen, zu deren Wellenbewegung das Randelement ds den hauptsächlichsten Beitrag liefert. Dies sind (vgl. S. 191) die Raumpunkte, die auf dem zu ds gehörigen Reflexionskegel liegen.

Leider bietet der ursprüngliche Kirchhoffsche Ansatz in dem jetzt betrachteten Ausnahmefalle, ebenso übrigens wie in dem Falle einer sehr engen oder auch allseitig sehr kleinen Beugungsöffnung, uns keine Handhabe ihn zu verbessern.

Es ist nun leicht eine ganze Klasse von Beugungsproblemen anzugeben, für die der Kirchhoffsche Ansatz im allgemeinen in allen Raumpunkten versagt. Dies tritt nämlich in allen Fällen ein, in denen der beugende Rand so verläuft, daß wenn auf einer von der Lichtquelle L ausgehenden Halbgeraden ein Bogenelement ds des beugenden Randes liegt, auf ihr oder in ihrer unmittelbaren Nähe mindestens noch ein zweites Bogenelement ds' des beugenden Randes zu finden ist. Dies findet statt, wenn bei entsprechendem Verlauf des beugenden Randes die Lichtquelle L eine solche Lage hat, daß das direkt einfallende Licht auf die beugende Öffnung streifend einfällt. In einem solchen Falle verschwindet ein zur Fortpflanzungsrichtung des einfallenden Lichtes senkrechter Querschnitt des Lichtkegels oder wird mindestens sehr eng oder auch allseitig sehr klein.

Dies ist aber auch stets der Fall, wenn die beugende Öffnung selbst sehr eng oder auch allseitig sehr klein ist. Wir umfassen somit diesen Fall und zugleich den oben besprochenen Fall des streifend einfallenden Lichtes, wenn wir feststellen, daß der Kirchhoffsche Ansatz nicht anwendbar ist, falls der zur Fortpflanzungsrichtung des einfallenden Lichtes senkrechte Querschnitt des Lichtkegels sehr eng oder auch allseitig sehr klein ist.

§ 2. Kann man in der Kirchhoffschen Beugungstheorie Schirme von beliebiger Gestalt verwenden?

Der Zweck, der zunächst folgenden Überlegungen ist der Nachweis, daß man auf sehr große Schwierigkeiten stößt, falls der flächenhafte Schirm S eine solche Gestalt hat, daß es von der Lichtquelle L ausgehende Halbgerade gibt, die ihn mehr als einmal schneiden. Um dies zu zeigen, sei angenommen, daß der beugende Schirm ursprünglich,

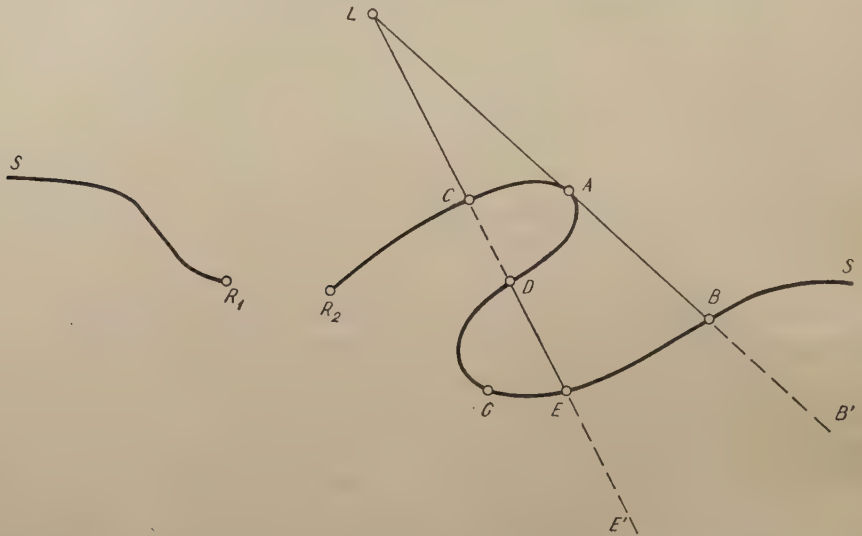


Fig. 1. Schematische Darstellung des Verlaufs der Kirchhoffschen Wellenbewegung bei der Beugung an einem „gewellten“ beugenden Schirme.

wie in § 1, nur eine einzige Beugungsöffnung hat, aber außerdem zum Teil so verläuft, daß es auch von der Lichtquelle L ausgehende Halbgerade gibt, die ihn mehr als einmal schneiden. In Fig. 1 ist ein solcher Schirm schematisch dargestellt. R_1 und R_2 bezeichnen die Schnittpunkte des beugenden Randes mit der Zeichenebene. Die von der Lichtquelle L ausgehende Halbgerade $LCDEE'$ hat mit dem Schirme S die drei Punkte C , D und E gemeinsam.

Gemäß den ursprünglichen Kirchhoffschen Annahmen (vgl. S. 66) hat man im Falle eines flächenhaften Schirmes S im Kirchhoff-Huygensschen Prinzip auf dem beleuchteten Teile S_0 des Schirmes S die Randwerte der direkt einfallenden Lichtwelle zu entnehmen, auf den übrigen Teilen des Schirmes S jedoch gleich null zu setzen. Der Wellenvorgang wird somit im ganzen unendlichen Raume durch den Kirchhoffschen Ansatz (vgl. S. 66):

$$u_K = \frac{e^{ikR}}{R} + \frac{1}{4\pi} \int_{S_0} \left\{ \frac{e^{ikr}}{r} \frac{\partial}{\partial n'} \left(\frac{e^{ik\varrho}}{\varrho} \right) - \frac{e^{ik\varrho}}{\varrho} \frac{\partial}{\partial n'} \left(\frac{e^{ikr}}{r} \right) \right\} df \quad (2.1)$$

gegeben. Hier bedeutet R , ebenso wie in § 1, den Abstand des Beobachtungspunktes P von der Lichtquelle L . Die Entfernung des Beobachtungspunktes P bzw. der Lichtquelle L von einem Flächenelemente df des beugenden Schirmes S_0 wird durch r bzw. ϱ bezeichnet. \mathbf{n}' ist die Normale an S_0 , die einen von der beleuchteten Seite von S_0 nach seiner beschatteten Seite weisenden Richtungssinn besitzt.

Da nach den in § 1 gemachten Voraussetzungen der Schirm S sich überall ins Unendliche erstreckt, so zerfällt der ganze unendliche Raum in zwei „Halbräume“, wenn wir S durch eine die beugende Öffnung überspannende Fläche F verschließen. Den Halbraum, in dem sich die Lichtquelle L befindet, wollen wir als den Licht-, den anderen als den Schatten-Halbraum bezeichnen.

Betrachten wir zunächst, der Einfachheit halber, den Fall, wo jede von der Lichtquelle L ausgehende Halbgerade den Schirm S nur einmal schneidet, so daß S_0 durch S gegeben wird. In diesem Falle kann man, wie Kirchhoff gezeigt hat (vgl. S. 67), den im ganzen Raume geltenden Ausdruck (2.1) in den nur im Schattenraume verwendbaren Ausdruck

$$u_r = \frac{1}{4\pi} \int_F \left\{ \frac{e^{ikr}}{r} \frac{\partial}{\partial n} \left(\frac{e^{ik\varrho}}{\varrho} \right) - \frac{e^{ik\varrho}}{\varrho} \frac{\partial}{\partial n} \left(\frac{e^{ikr}}{r} \right) \right\} df \quad (2.2)$$

umformen. Die Normale \mathbf{n} an die Fläche F besitzt einen von dem Schattenhalbraum in den Lichthalbraum weisenden Richtungssinn.

Nehmen wir zunächst die Kirchhoffsche Vorschrift als ausnahmslos bindend an, daß die Integration im ursprünglichen Kirchhoffschen Ansatz (2.1) über S_0 zu erstrecken ist, und betrachten die Folgerungen, die sich in dem Falle ergeben, wo der beugende Schirm S den in der Fig. 1 angedeuteten Verlauf hat. Es kann dann zwar der ursprüngliche Kirchhoffsche Ansatz (2.1) in den Ausdruck (2.2) umgeformt werden, die Integration in (2.2) ist dann aber nicht nur über die als gegeben angenommene Beugungsöffnung F , sondern im allgemeinen auch noch über weitere Beugungsöffnungen F_i ($i = 1, 2, \dots$) zu erstrecken. Die beugenden Ränder dieser letzteren beugenden Öffnungen werden dabei durch Schnittkurven der Schirmfläche S mit Kegelflächen gegeben, deren Scheitel in der Lichtquelle L liegen und die so verlaufen, daß ihre Erzeugenden den Schirm S berühren (vgl. in Fig. 1 z. B. die Erzeugende $LABB'$). Jede Beugungsöffnung F_i ist so beschaffen, daß auf sie, wie in § 1 angegeben, das Licht der Lichtquelle L derart streifend einfällt, daß der entsprechende Lichtkegel gerade verschwindet. Der gesamte durch den Kirchhoffschen Ansatz gegebene Wellenvorgang besteht dann aus der Superposition der durch die Beugungsöffnung F sowie alle Beugungsöffnungen F_i gegebenen Wellenbewegungen (*Unabhängigkeitstheorem für die Beugungsöffnungen*, vgl. S. 85).

Aus der Tatsache, daß der Kirchhoffsche Ansatz die den einzelnen Beugungsöffnungen F_i entsprechenden Wellenzustände nicht in Übereinstimmung mit der Wirklichkeit beschreibt, folgt unausweichlich, daß die oben angegebene Wellenbewegung nicht als eine Näherung eines Wellenvorganges angesehen werden kann, der

irgendwie physikalisch realisierbar ist. Sieht man den Schirm als undurchsichtig an, so hat es selbstverständlich keinen Sinn anzunehmen, daß die von den Beugungsöffnungen F_i stammende Wellenbewegung auch im Schattenhalbraum des Schirmes S sich geltend macht. Es ist aber auch ganz unzulässig die Beiträge der Beugungsöffnungen F_i zum Kirchhoffschen Ansatz (2.2) im Lichthalbraum des Schirmes S zu berücksichtigen, da sie doch nicht korrekt die durch die einzelnen Beugungsöffnungen F_i verursachten Wellenbewegungen wiedergeben.

Aus den obigen Überlegungen folgt somit, daß die Kirchhoffsche Vorschrift, die Integration sei nur über den Teil S_0 des Schirmes S zu erstrecken, in allen jenen Fällen nicht anwendbar ist, in denen als Folge dieser Vorschrift Beugungsöffnungen von der Art der Beugungsöffnungen F_i auftreten.

Setzen wir nun voraus, daß der Schirm S undurchsichtig ist und stellen uns die Aufgabe, die durch die Beugungsöffnung F verursachten Beugungserscheinungen in der Nähe der Schattengrenze dieser Beugungsöffnung zu beschreiben. Es wird dann im allgemeinen genügen, ohne Rücksicht darauf wie der Schirm S verläuft, im Schattenhalbraum nur die Wellenbewegung zu berücksichtigen, die gemäß dem Kirchhoffschen Ansatz von der Beugungsöffnung F beigesteuert wird. Falls jedoch der Schirm S , wie die Fig. 1 es andeutet, gewellt ist, so begegnen wir sogleich wieder Schwierigkeiten wenn wir versuchen, diese Wellenbewegung regulär gemäß der Schwingungsgleichung $\Delta u + k^2 u = 0$ durch die Beugungsöffnung F hindurch in den Lichthalbraum fortzusetzen.

Um diese Schwierigkeiten zu erklären, bemerken wir zunächst, daß ohne Rücksicht auf die Gestalt des Schirmes die reguläre Fortsetzung der Lösung im Schattenhalbraume durch die Beugungsöffnung F hindurch im Lichthalbraume in Übereinstimmung mit (1.1) wieder aus der gemäß der geometrischen Optik sich fortpflanzenden direkt einfallenden Lichtwelle und der vom beugenden Rande B der Beugungsöffnung F ausgehenden Beugungswelle besteht.

Dieser Tatbestand ermöglicht zunächst, ohne Rücksicht auf die Gestalt des Schirmes S , das mathematische Verhalten anzugeben, das die in der Kirchhoffschen Theorie auftretenden Schirme charakterisiert. Aus ihm folgt nämlich, daß die Wellenbewegung in dem Schirme S (vgl. S. 108) einen Sprung um die direkt einfallende Lichtwelle erleidet. Da die Beugungswelle somit stetig durch die Schirmfläche hindurchgeht, so ist der in der Kirchhoffschen Theorie auftretende Schirm physikalisch dadurch ausgezeichnet, daß er für die Beugungswelle vollständig durchsichtig ist (vgl. S. 114).

Kehren wir nun zur Betrachtung des Falles zurück, wo der Schirm S eine gemäß der Fig. 1 gewellte Gestalt besitzt und betrachten die Wellenbewegung längs der von der Lichtquelle L ausgehenden Halbgeraden $LCDEE'$, die den Schirm S mehrmals schneidet. Auf den Strecken LC , CD und EE' findet man dann Wellenvorgänge, die mit unseren Erwartungen im Einklange stehen, falls wir uns damit abfinden, daß der Kirchhoffsche Schirm für die Beugungswelle durchsichtig ist. Man bemerkt insbesondere, daß auf den gestrichelten Strecken CD und EE' keine direkt einfallende

Lichtwelle auftritt, so daß man aus diesem Grunde den Schirm S als für die direkt einfallende Lichtwelle vollständig undurchsichtig bezeichnen könnte. Nicht im Einklang mit dieser Feststellung befindet sich jedoch die Wellenbewegung auf der Strecke DE . Hier tritt nämlich außer der Beugungswelle noch die direkt einfallende Lichtwelle auf, während wir uns hier doch in Raumpunkten befinden, in denen der geometrischen Optik zufolge Schatten bestehen sollte.

Der beschrittene Ausweg ist somit nicht gangbar. Will man in dem Raumgebiet $ADGEB$ einen Schatten haben, so kann man dies erzielen, falls man neben F noch eine Beugungsöffnung F_1 im Schirme S einführt, zu deren beugendem Rande die Punkte A und B gehören. Da jedoch F_1 eine Beugungsöffnung darstellt, für die der Kirchhoffsche Ansatz versagt, kommt man auf diese Weise auf den vorhin betrachteten Fall zurück.

Aus den obigen Überlegungen folgt, daß man im Falle eines beugenden Schirmes, der von den von der Lichtquelle ausgehenden Halbgeraden auch in mehr als einem Punkte geschnitten wird, auf Grund des Kirchhoffschen Ansatzes keine Wellenbewegung angeben kann, die den Wellenvorgang im ganzen Raume befriedigend darstellt. Will man also die bei der Beugung auftretende Wellenbewegung mit Hilfe des Kirchhoffschen Ansatzes im ganzen Raume beschreiben, so muß man sich auf beugende Schirme beschränken, die jede von der Lichtquelle L ausgehende Halbgerade höchstens in einem Punkte schneidet.

Aber auch solche Schirme weisen, falls sie nicht eben sind, immer noch sozusagen einen Schönheitsfehler auf (vgl. S. 114). Bei nicht ebenen Schirmen kann man ja feststellen, daß durch sie die Beugungswelle ungestört hindurchgeht. In einem solchen Falle kann man nämlich stets von den Punkten des beugenden Randes ausgehende Halbgerade angeben, die den beugenden Schirm in einem nicht auf dem beugenden Rande liegenden Punkte schneiden. Nur ebene Schirme sind dadurch ausgezeichnet, daß man nicht gezwungen ist, sie als durchsichtig für die Beugungswelle anzusehen. Da sie auch für die direkt einfallende Lichtwelle undurchsichtig sind, kann man sie als schwarz betrachten. Hat aber der in der Kirchhoffschen Beugungstheorie auftretende Schirm (z. B. im Falle wo der beugende Rand durch eine Raumkurve gegeben wird) eine andere Gestalt, so ist es geraten, um eine Verwirrung zu vermeiden, ihn als einen Kirchhoffschen Beugungsschirm zu bezeichnen (vgl. S. 69).

Aus diesen Überlegungen soll man jedoch nicht den Schluß ziehen, daß die Kirchhoffsche Theorie nur zur Darstellung der Beugungserscheinungen an ebenen Schirmen brauchbar ist. Im allgemeinen wird sie nämlich die Beugungserscheinungen im Schattenraume vor allem in der Nähe der Schattengrenze, wo sie am markantesten auftreten, befriedigend darstellen, auch wenn der Schirm S nicht eben ist, d. h. wenn der beugende Rand durch eine Raumkurve gegeben wird.

КРАТКОЕ СОДЕРЖАНИЕ

А. Рубинович. Незамеченный до сих пор случай, в котором нельзя применять интеграл Кирхгофа для описания явления диффракции.

На основании некоторой теоремы о независимости для волны диффракции Кирхгофа, исследовано границу применимости волнового движения определенного интегралом Кирхгофа для описания явления диффракции. Оказалось, что интеграл Кирхгофа неприменим не только — как известно — для очень малых или очень узких отверстий, но также в случае, когда край диффракции имеет такую форму, что существуют полупрямые выходящие из источника света, которые проходят точно или приближенно через две точки лежащие на разных частях огибающего края. Рассмотрено следствия отсюда вытекающие для формы экранов допустимых в теории Кирхгофа диффракции света.

NUCLEON-SURFACE INTERACTION AND THE (p, n) REACTIONS

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(Received April 15, 1957)

The contribution is discussed to the diff. cross-section for (p, n) reaction (as calculated according to the assumption of the direct n -interaction) due to the nucleon-surface interactions of the Bohr & Mottelson type. The effective contribution to the neutron-proton potential due to the proton-core (surface) — neutron coupling and the proton (neutron) — surface selfaction couplings are calculated. This correction being of the second order in the B.—M. coupling constant appear as a part of the total (p, n) transition operator. The Coulomb effect of the incident proton wave is taken into account. The relative contribution of the correction terms to the diff. cross-section for the $^{28}\text{Si}(p, n)^{29}\text{P}$ angular distribution is small.

§ 1. Introduction

Recently (Sawicki, 1956¹) the angular distributions and the neutron polarization of the neutrons from (p, n) reactions were calculated under the assumption that a direct mechanism of the type as proposed by Austern et al. (1953) is the primary mechanism operative in a (p, n) reaction. This mechanism dominates over the compound nucleus formation in a number of particular cases, when we are dealing with a reaction far away the pronounced resonances of the excitation curve and for nuclei containing one outer nucleon (or a few nucleons) the most loosely bound with a double magic (or with closed subshells) core. It applies, before all, to sufficiently small energies² of the incident protons, when the only neutron that can be knocked out from the nucleus the outer one.

Following Austern et al. (1953) and similarly as in I we assume that the neutron which is initially the most loosely bound (with a spin-zero core) and which is in a state of total angular momentum j_i , orbital angular momentum l_i and z-component m_i , is knocked out from the surface of the nucleus by the incoming proton which is then

¹ further referred to as I.

² one must remember, however, that the energy has to be sufficiently high (5—15 MeV) to neglect the compound nucleus formation important at small energies.

captured in to a state of total angular momentum j_f , orbital angular momentum l_f and z-component m_f .

It was assumed in I that the knock-out mechanism is due to the interaction of the incident proton with the target neutron i.e. the potential V_{np} . It seems, therefore, interesting to investigate the contribution to the reaction from the interactions of both the nucleons with the surface of the core in the sense of the Bohr-Mottelson model.

In the case of target nuclei considered here (one or a few nucleons outside the core) the equilibrium deformations of the core are expected to be rather small (almost spherical nucleus). Only vibrational excitations of the surface should, therefore, contribute. That means that the rotational excitations of the target nucleus are to be neglected. In this situation the weak coupling approximation for the nucleon-surface interaction is applicable. The contributions to the (p, n) transition operator due to these interactions consists then of an additional proton — neutron interaction via virtual phonon excitations of the surface plus similar proton (neutron) selfaction terms. These interactions are of the type of particle-core (surface) — particle couplings i.e. interactions of the 2nd order in the coupling constant.

§ 2. Calculations

The neutron and the proton are assumed to interact with the surface via the usual interactions (in the notation of Bohr 1952, Bohr & Mottelson 1953):

$$H_{\text{int}}^{(p)}(\vec{r}_p, \alpha_\mu) = -V_0^{(p)} R_0 \delta(r_p - R_0) \sum \alpha_\mu Y_{2\mu}(\hat{\Omega}_p) \quad (1a)$$

$$H_{\text{int}}^{(n)}(\vec{r}_n, \alpha_\mu) = -V_0^{(n)} R_0 \delta(r_n - R_0) \sum \alpha_\mu Y_{2\mu}(\hat{\Omega}_n) \quad (1b)$$

$$H_{\text{int}} = H_{\text{int}}^{(p)} + H_{\text{int}}^{(n)} \quad (2)$$

where $V_0^{(p)}$, $V_0^{(n)}$ are the square well depths appropriate to the bound proton and neutron³.

All the particle-core (surface) — particle couplings are to be written in the form of the (second order perturbation) operator:

$$\Delta V = \sum \frac{H_{\text{int}} |H'_0 \alpha' \rangle \langle \alpha' H'_0| H_{\text{int}}}{E_0 - H'_0} \quad (3)$$

where E_0 is the total energy of the system in the initial and final states, and $|H'_0 \alpha' \rangle$ denotes an eigenket of the unperturbed hamiltonian:

$$H_0 = H_{\text{surface}} + T_n + T_p + V_n + V_p \quad (4)$$

where H_{surf} is the hamiltonian of the free surface; and $T_p(T_n)$ denote the kinetic and potential energies of the proton (neutron), respectively.

The energy H'_0 of an intermediate state is the sum of the proton energy $H_0^{(p)}$

³ this point is discussed below.

the neutron energy $H_0^{(n)}$ and the phonon energy $= \hbar\omega$ (there are only one phonon transitions involved).

On neglecting $H_0^{(p)}$ and $H_0^{(n)}$ as compared with $\hbar\omega$ one obtains (see e.g. Bohr & Mottelson 1953, Ford & Levinson 1955) the simplified operator:

$$\Delta V = \frac{H_{int}^2}{E_0 - \hbar\omega} \quad (5)$$

However, our binary rearrangement collision is not the case and Eq. (5) is not valid.

The (p, n) reaction amplitude is calculated according to I in the spirit of Tobocman's (1954) theory with the only difference that the transition operator V_{np} is replaced by

$$V_{np} + \Delta V$$

For the sake of numerical computations we shall confine ourselves to the bound states S (i. e. $l_i = l_f = 0$) where the spin-orbit coupling does not operate. To simplify computations the spin-orbit coupling will be neglected in the V_p and V_n potentials. The general case is discussed in Appendix I.

The initial state of the system corresponding to our scattering problem is:

$$|E_0; i\rangle = |000\rangle \cdot \Psi_i[\mu_i] \cdot \Psi_p[\mu_p] \quad (6)$$

where $|000\rangle \equiv |N=0, R=0, m_R=0\rangle$ denotes the unperturbed state of the surface and the wave function of the bound state of the neutron is assumed according to I in the form:

$$\Psi_i[\mu_i] = R_0^{-\epsilon_i}(r_n) \cdot Y_{00}(\Omega_n) \cdot \chi_{\mu_i}(\sigma_n) \quad (7)$$

and the incident proton wave is:

$$\Psi_p[\mu_p] = \sum_{L_p M_p} b^*(L_p, M_p) R_{L_p}^{E_0 + \epsilon_i}(r_p) \cdot Y_{L_p M_p}(\Omega_p) \cdot \chi_{\mu_p}(\sigma_p) \quad (8)$$

The final state "equivalent" in the sense of Tobocman's theory may be written as:

$$\langle E_0; f | = \langle 000 | \cdot \Psi_f^*[\mu_f] \cdot \Psi_n^*[\mu_n] \quad (9)$$

where

$$\Psi_f^*[\mu_f] = R_0^{*- \epsilon_f}(r_p) Y_{00}^*(\Omega_p) \chi_{\mu_f}^*(\sigma_p) \quad (10)$$

denotes the bound state of the proton and

$$\Psi_n[\mu_n] = \begin{cases} 0 & \text{for } r_n < R_0 \\ \sum_{LM_L} a(L, M_L) R_L^{*E_0 + \epsilon_f}(r_n) \cdot Y_{LM_L}(\Omega_n) \cdot \chi_{\mu_n}^*(\sigma_n) & \text{for } r_n \geq R_0 \end{cases} \quad (11)$$

is the outgoing neutron wave. The "Tobocman radius" is assumed to be the nuclear radius R_0 ($R_0 = 1.45 \times A^{1/3} \cdot 10^{-13}$ cm).

The intermediate states are:

$$|H_0, \alpha' \rangle = |NR m_R \rangle \Psi[\mu'_p] \cdot \Psi[\mu'_n] \quad (12)$$

where

$$\Psi[\mu'_p] = R_{l'_p}^{H_0^{(p)}}(r_p) \cdot Y_{l'_p m'_p}(\Omega_p) \cdot \chi_{\mu'_p}(\sigma_p) \quad (13)$$

$$\Psi[\mu'_n] = R_{l'_n}^{H_0^{(n)}}(r_n) \cdot Y_{l'_n m'_n}(\Omega_n) \cdot \chi_{\mu'_n}(\sigma_n) \quad (14)$$

The summation over all the intermediate states $\sum_{\alpha' H_0'}$ is to be understood as the operator:

$$\int dH_0^{(p)} \int dH_0^{(n)} \int dH_0' \sum_{NRm_R} \sum_{l'_p m'_p \mu'_p} \sum_{l'_n m'_n \mu'_n} \delta(H_0' - H_0^{(p)} - H_0^{(n)} - N\hbar\omega) \quad (15)$$

After performing all the angular spin- and others intergrations and summations, making use of the properties of the operators α_μ the well known formula for the products of two spherical harmonics, the properties of the vector addition coefficients and various orthogonality relations we finally obtain the correction to the reaction amplitude due to the operator ΔV in the form:

$$\begin{aligned} \langle E_0; f | \Delta V | E_0; i \rangle &\equiv \Delta M(\mu_p \mu_i \rightarrow \mu_f, \mu_n) \\ &= \delta_{\mu_p \mu_f} \delta_{\mu_i \mu_n} \{ \Gamma_{np}^2 (Z_{AD} + Z_{BC}) \Phi_1 + (\Gamma_p^2 Z_{AC} + \Gamma_n^2 Z_{BD}) \Phi_2 \} \end{aligned} \quad (16)$$

Where $\Gamma_{np}^2 = \Gamma_n \Gamma_p$, $\Gamma_n = V_0^{(n)} R_0^3 \sqrt{\frac{\hbar}{2B\omega}} \frac{1}{\sqrt{4\pi}}$, $\Gamma_p = V_0^{(p)} R_0^3 \sqrt{\frac{\hbar}{2B\omega}} \frac{1}{\sqrt{4\pi}}$

($B \equiv B_2$ — the mass coefficient of the collective motion)

$$\Phi_1 = \Phi_1(\Theta) = \sum_{m_R=-2}^2 a(2, m_R) b^*(2, m_R) = 5\pi (3 \cos 2\Theta + 1) \quad (17a)$$

$$\Phi_2 = 20\pi \quad (17b)$$

$$\begin{aligned} Z_{AD} &= R_0^{*- \varepsilon_f}(R_0) \cdot R_2^{H_0^{(p)}=E_0+\varepsilon_i}(R_0) \cdot R_2^{H_0^{(n)}=E_0+\varepsilon_f}(R_0) \cdot R_0^{-\varepsilon_i}(R_0) \times \\ &\times (\hbar\omega - E_0 - \varepsilon_f - \varepsilon_i)^{-1} \end{aligned} \quad (18a)$$

$$\begin{aligned} Z_{BC} &= R_2^{*E_0+\varepsilon_f}(R_0) \cdot R_0^{H_0^{(p)}=-\varepsilon_i}(R_0) \cdot R_0^{*H_0^{(p)}=-\varepsilon_f}(R_0) \cdot R_2^{E_0+\varepsilon_i}(R_0) \times \\ &\times (-\hbar\omega + E_0 + \varepsilon_f + \varepsilon_i)^{-1} \end{aligned} \quad (18b)$$

$$\begin{aligned} Z_{AC} &= R_0^{*- \varepsilon_f}(R_0) R_0^{E_0+\varepsilon_i}(R_0) \left\{ \int_{R_0}^{\infty} dr_n \cdot r_n^2 \cdot R_0^{*E_0+\varepsilon_f}(r_n) R_0^{-\varepsilon_i}(r_n) \right\} \times \\ &\times \left\{ \int_0^{\infty} \frac{dH_0^{(n)} | R_2^{H_0^{(p)}}(R_0) |^2}{E_0 - H_0^{(p)} + \varepsilon_f - \hbar\omega} \right\} \end{aligned} \quad (18c)$$

$$Z_{BD} = R_0^{*E_0+\varepsilon_f}(R_0) \cdot R_0^{-\varepsilon_i}(R_0) \left\{ \int_0^\infty dr_p r_p^2 R_0^{*- \varepsilon_f}(R_0) R_0^{E_0+\varepsilon_i}(r_p) \right\} \times \\ \times \left\{ \int_0^\infty \frac{dH_0^{(n)}}{E_0 - H_0^{(n)} + \varepsilon_f - \hbar\omega} |R_2^{H_0^{(n)}}(R_0)|^2 \right\} \quad (18d)$$

On calculating Z_{AD} and Z_{BC} use has been made of approximate relations:

$$\int_{R_0}^\infty dr_n \cdot r_n^2 R_2^{*E_0+\varepsilon_f}(r_n) \cdot R_2^{H_0^{(n)}}(r_n) \approx \delta(E_0 + \varepsilon_f - H_0^{(n)}) \quad (19a)$$

$$\int_0^\infty dr_p r_p^2 R_2^{*H_0^{(p)}}(r_p) R_2^{E_0+\varepsilon_i}(r_p) \approx \delta(E_0 + \varepsilon_i - H_0^{(p)}) \quad (19b)$$

The justification of these approximations (the former (19a) being the more drastic one) is the assumption that if the waves $l = 2$ being nearly free can be approximated by the spherical Bessel functions (or their Coulomb analogues).

From Eq. (18) one readily sees that Eq. (5) would be completely unreliable (different denominators in different terms). Due to the coupling by the spherical harmonics all the sums over $L_p, M_p, L, M_L, l_n, m_n, l_p, m_p$ reduce to a finite number of terms.

§ 3. Numerical Results and Calculations

The $^{29}\text{Si}(p, n)^{29}\text{P}$ reaction ($l_i = l_f = 0$) is considered similarly as in I. The binding energies are $\varepsilon_i = 8.194$ MeV; $\varepsilon_f = 2.691$ MeV; $E_0 = -2.194$ MeV corresponds to the energy of the incident protons $E_p = 6$ MeV calculated according to Bohr (1952) = 4.955 MeV. The Coulomb wave function $R_0^{-\varepsilon_p}(r_p)$ was approximated as in I by an "equivalent neutron" function. For the sake of only a rough estimation the nuclear interactions (scattering terms) were neglected in the waves of free nucleons. The integrals occurring in Z_{BD} and Z_{AC} were computed, in part, numerically⁴.

The numerical computations were performed in two cases: 1° disregarding the Coulomb effect of the incident proton wave, 2° including Coulomb effect.

To estimate the relative contribution of the correction considered herein to the (p, n) process according to I the main part of the reaction amplitude was taken to be:

$$\langle E_0, f | V_{np} | E_0, i \rangle = M(\mu_p, \mu_i \rightarrow \mu_f, \mu_n) \quad (20)$$

V_{np} being of the form: $V_{np} = (V_1 + V_2 \vec{\sigma}_n \vec{\sigma}_p) \delta(\vec{r}_n - \vec{r}_p)$. For the numerical estimation V_{np} was taken to be:

$$V_{np} = \frac{4\pi\hbar^2}{M} \delta(\vec{r}_n - \vec{r}_p) \left[\frac{a_1 + a_0}{2} + \frac{a_1 - a_0}{2} P_\sigma \right] \quad (21)$$

⁴ this point will be discussed below.

where $a_1 = 4.31 \times 10^{-13}$ cm and $a_0 = -24.34 \times 10^{-13}$ cm are the triplet and the singlet $n-p$ scattering lengths, respectively, and $P_\sigma = \frac{1}{2}(1 + \vec{\sigma}_n \cdot \vec{\sigma}_p)$. Hence:

$$M(\mu_p, \mu_i \rightarrow \mu_f, \mu_n) = M_{00} \left\{ \frac{a_1 + a_0}{2} \delta_{\mu_f \mu_p} \delta_{\mu_i \mu_n} + \frac{a_1 - a_0}{2} \delta_{\mu_i \mu_f} \cdot \delta_{\mu_p \mu_n} \right\} \quad (22)$$

where M_{00} is given in I.

The angular distribution is given by:

$$\sum_{\mu_n \mu_i} \sum_{\mu_f \mu_p} |M(\mu_p, \mu_i \rightarrow \mu_f, \mu_n) + \Delta M(\mu_p, \mu_i \rightarrow \mu_f, \mu_n)|^2 = \alpha(\Theta) \quad (23)$$

The numerical values of the relative contributions of the operator ΔV are given by:

$$x = \frac{\alpha(\Theta) - \alpha_0(\Theta)}{\alpha_0(\Theta)} \quad (24)$$

where

$$\alpha_0(\Theta) = \sum_{\mu_n \mu_i} \sum_{\mu_f \mu_p} |M(\mu_p, \mu_i \rightarrow \mu_f, \mu_n)|^2 \quad (25)$$

The Born approximation introduces large overestimates of the selfaction terms Z_{AC} and Z_{BD} . In this approximation $x(\Theta = 0)$ for the cases 1 and 2 are 4.25% and 12.04%, respectively maximum x being 20% at the minimum of $\alpha_0(\Theta)$. The correction $x\alpha_0(\Theta)$ due to ΔV is nearly isotropic.

If one used the more correct distorted wave method like that of Lamarsh & Feshbach (1956), one would find Z_{AC} and Z_{BD} very small (due to the quasiorthogonality of the radial wave functions occurring in Z_{AC} and Z_{BD} corresponding to the shell model and optical model square wells). One would then have $x(\Theta = 0) \approx -0.2\%$ (in the case 1°), the correction $x\alpha_0(\Theta)$ due to ΔV being of the form: $const_1 + const_2 \cdot \cos 2\Theta$.

The correction due to ΔV increases the diff. cross-section by a small amount. The numerical results are to be trusted only rather qualitatively because of great uncertainty in the numerical values of the constant coefficients in and the values $V_0^{(p)}$, $V_0^{(n)}$. The latter were assumed to be the square well depths corresponding to the bound states of the outer nucleons, while Brink (1955) an optical model square well for the neutron inelastically scattered from a heavy nucleus. On the other hand, Hayakawa & Yoshida (1955) use square wells appropriate to bound states for the scattering of protons from ^{24}Mg .

It seems possible that the most reasonable choice would be to use bound state square wells for those terms of Eq. (16) where the respective $H_{int}^{(n,p)}$ operate on bound states and to use optical model square wells when operating on free scattering states. This should increase the effect of ΔV .

The authors are indebted to Dr. M. Günther for a helpful discussion.

Appendix I.

The Distortion of the Proton and Neutron Waves by a Spin-Orbit Potential

The effect of the introduction of an $\vec{L} \cdot \vec{S}$ coupling to the potentials V_p and V_n results in the replacement of $\Psi_p [\mu_p]$ (Eq. (8)) by:

$$\Psi_p [\mu_p] = \sum_{L_p M_p} \sum_{J_p M_{J_p}} b^* (L_p, M_p) (L_p \frac{1}{2}; M_p \mu_p | J_p M_{J_p}) R_{L_p}^{E_0 + \epsilon_i} (r_p) J_{J_p L_p \frac{1}{2}}^{M_{J_p}} (\Omega_p, r_p) \quad (A_1^1)$$

in the usual notation (see e.g. I) and $\Psi_n [\mu_n]$ for $r_n \geq R_0$

$$\Psi_n [\mu_n] = \sum_{L_M L} \sum_{J_M J} a (L, M_L) (L \frac{1}{2}; M_L \mu_n | J M_J) R_{L_J}^{E_0 + \epsilon_f} (r_n) \cdot J_{J, L, \frac{1}{2}}^{M_J} (\Omega_p, \sigma_p) \quad (A_1^2)$$

Similarly the intermediate states to be substituted for $\Psi [\mu_p']$, $\Psi [\mu_n']$ are:

$$\Psi [\mu_p'] = R_{j_p' L_p'}^{H_0^{(p)}} (r_p) Y_{j_p' L_p' \frac{1}{2}}^{\mu_p'} (\Omega_p, \sigma_p) \quad (A_1^4)$$

$$\Psi [\mu_n'] = R_{j_n' L_n'}^{H_0^{(n)}} (r_n) Y_{j_n' L_n' \frac{1}{2}}^{\mu_n'} (\Omega_n, \sigma_n) \quad (A_1^5)$$

The results of the calculations are much more complicated, but the amplitude $\Delta M (\mu_p \mu_i \rightarrow \mu_f \mu_n)$ contains also only a finite number of terms. For example the analogue of the expression $Z_{BC} \cdot \Phi_1 \delta_{\mu_p \mu_f} \cdot \delta_{\mu_i \mu_n}$ is:

$$\frac{\sqrt{4\pi} R_0^{-\epsilon_i} (R_0) R_0^{*- \epsilon_f} (R_0)}{\hbar\omega - \epsilon_i - \epsilon_f - E_0} \sum_{L J L_p J_p M_p} \alpha_{JL}^* \beta_{J_p L_p} (-1)^{\mu_f - M - \mu_p} b (L_p M_p) \times \\ \times a (L, M - \mu_f - \mu_n + \mu_i) (L_p \frac{1}{2} M \mu_p | J_p M + \mu_p) (J_p 2M + \mu_p, \mu_f - M_p - \mu_p | \frac{1}{2} \mu_f) \times \\ \times (L \frac{1}{2} M - \mu_f - \mu_n + \mu_i \mu_n | J, M - \mu_f + \mu_i) (\frac{1}{2} 2 \mu_i M - \mu_f | J M - \mu_f + \mu_i)$$

where

$$\alpha_{JL}^* = R_{JL}^{*E_0 + \epsilon_f} (R_0) (-1)^{J - \frac{1}{2}} \sqrt{\frac{5}{4\pi}} \sqrt{2} W (\frac{1}{2}, 0, J, L | \frac{1}{2}, 2) (0 200 | L 0) \\ \beta_{JL} = R_{J_p L_p}^{E_0 + \epsilon_i} (R_0) \sqrt{\frac{5}{4\pi}} \sqrt{(2L_p + 1)(2J_p + 1)} W (y_p L_p \frac{1}{2} 0 | \frac{1}{2} 2) (L_p 200 | 00) \quad (A_1^5)$$

The last vector addition coefficient occurring in (A₁⁵) admits J to be only 3/2 or 5/2. Hence $L = J + \frac{1}{2} = 1, 2, 3, 4$. Similarly the summations over $L_p J_p$ are confined to four terms: $(L_p = 1, J_p = \frac{3}{2})$, $(L_p = 2, J_p = \frac{3}{2})$, $(L_p = 2; J_p = \frac{5}{2})$, $(L_p = 3, J_p = \frac{5}{2})$

To calculate (A₁⁵) one has only to compute a finite number of terms.

Appendix II

The Neutron Polarization

The neutron polarization was calculated in I under the assumption that the final state neutron scatters in a spin-orbit potential. One would like to know how ΔV affects this polarization. Even if one, inconsistently, neglects the spin-orbit coupling in ΔM one can realise the order of magnitude and the sign of the correction to the polarization P given by:

$$\frac{\Delta P}{P} \approx \frac{3a_1 + a_0}{\frac{3}{4}a_1^2 + \frac{1}{4}a_0^2} \left\{ \frac{\operatorname{Re} \{ \Delta M (M_{00}^*(+) - M_{00}^*(-)) \}}{|M_{00}(+)|^2 - |M_{00}(-)|^2} - \frac{\operatorname{Re} \{ \Delta M (M_{00}^*(+) - M_{00}^*(-)) \}}{|M_{00}(+)|^2 + |M_{00}(-)|^2} \right\} \quad (A_{II}1)$$

The influence of ΔV on P was found very small.

КРАТКОЕ СОДЕРЖАНИЕ

Е. Савицкий, З. Шиманский, *Взаимодействие нуклонов с поверхностью и реакция (p, n).*

Обсуждается поправку дифференциального эффективного сечения на реакцию (p, n) происходящую от взаимодействия нуклонов с поверхностью, согласно модели Бора и Мотельсона. Подсчитано эффективный потенциал нейтрон-протон, происходящий от сопряжения протон-остов (поверхность) нейтрон, а также соответствующие члены взаимодействия. Эти потенциалы являются поправками к целому оператору переходов (p, n). Учтено кулоновский эффект падающей протоновой волны. Относительный вклад этих эффектов в эффективное сечение на реакцию $^{28}\text{Si}(p, n)^{28}\text{P}$ является малым.

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INVESTIGATION OF INFRARED ABSORPTION IN ALKALI HALIDE CRYSTALS WITH ANIONIC IMPURITIES

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(Received April 23, 1957)

The infrared absorption by KBr, KCl and KJ monocrystals containing a small amount of impurities (of the order of 10^{-2} mol %) of KNO_3 , K_2CO_3 , etc. was investigated. It is known that the introduction of the impurities results in the appearance of absorption bands in the infrared. It was shown that some of these bands undergo change when the crystals are heated and cooled rapidly, others change when irradiated by ultraviolet.

The change of absorption with temperature was investigated.

In the case of crystals containing KNO_3 it was possible to determine the NO_2^- and NO_3^- ion content by polarographic methods. It was also possible to determine the number of centres responsible for absorption in two well-separated bands arising after the addition of KNO_3 or KNO_2 .

The results of the polarographic measurements were compared with the data obtained on the basis of infrared absorption investigations.

Introduction

It is known that alkali halide crystals are quite transparent in the near infrared and first begin to absorb in the so-called residual ray region, which for these crystals, consists of a range in the far infrared. Absorption in this region is connected with the vibrations of ions situated at the lattice points. If into a crystal of this type we introduce as impurities anions consisting of several atoms (e. g. CO_3^{2-} , NO_3^- , SO_4^{2-} , etc.), then in the short wave region of the infrared there appear new absorption bands connected with the internal vibration of the anions introduced into the lattice.

In particular, if we grow KBr, KCl, or KJ monocrystals with impurities of K_2CO_3 or KNO_3 , then absorption bands appear in the infrared at 7μ and 8μ . For crystals containing KNO_3 these bands were found by Maslakowicz (1928), the bands at 7μ being ascribed to NO_3^- molecules and the bands at 8μ being ascribed to NO_2^- molecules. Very striking is the observation by Wardzyński (1955), namely, that among the absorption bands in the cases of CO_3^{2-} and NO_3^- anions we find bands vanishing according to the amount of irradiation of the sample by ultraviolet and bands which grow stronger during irradiation. When the monocrystals whose absorption was changed by being

irradiated are heated nearly to their melting point the absorption returns to initial state. These facts require further investigation in order to gather the widest possible experimental data which could eventually provide an explanation of the observed phenomena.

In this paper we are concerned primarily with the absorption bands at 7μ and 8μ for KBr and KCl monocrystals small impurities of K_2CO_3 and KNO_3 . Since the actual quantity of NO_3^- and NO_2^- ions in the samples can be determined by the polarographic method, the main attention was paid to monocrystals containing KNO_3 . The monocrystals were grown by the Kyropoulos (1926) method from the melted mass. Slabs of the required size and thickness may be obtained from the clusters by cutting along the cleavage planes. The surfaces thus obtained were good enough to allow measurement of the transmission without any additional polishing.

I. Measurement of the Transmission of the Crystals in the Infrared

The transmission measurements in the infrared region at 7μ were made with a double-beam Hilger D-209 spectrometer provided with a NaCl prism. The spectrometer

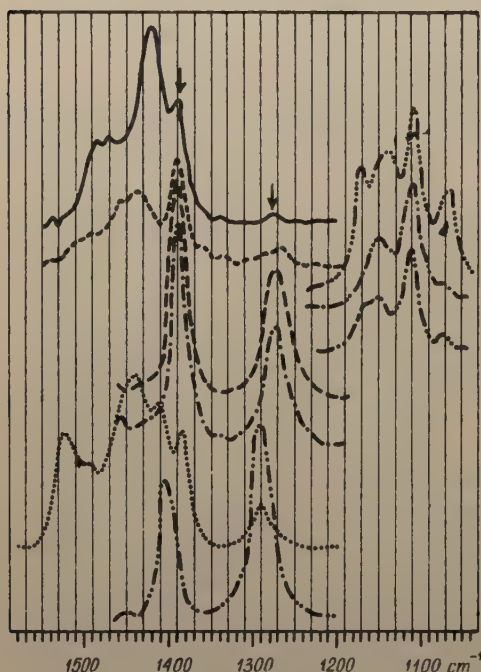


Fig. 1. Absorption of KBr and KCl monocrystals with different anionic impurities

— KBr KOH	— KBr K_2SO_4	— KCl KNO_3
- - - KBr KON_3	- - - KBr K_2CO_3	- - - KBr Na_2SO_4
... KCl KOH	- · - KBr KNO_2	- · - KBr $Na_2S_2O_5$

was connected to a recording apparatus. Owing to a special linkage arrangement for rotating the prism in the spectrometer, equal intervals of the spectra measured in wave numbers correspond to equal segments of the curve on the recording paper. During the measurements a prism of sodium chloride was used. A Nernst burner was used as a light source. The spectrometer slit width could be changed automatically to compensate for changes in intensity resulting from the spectral distribution of the source. The slit width used during the measurements varied between 0.2 — 0.3 mm. The dispersion curve was drawn on the basis of data on the absorption of polystyrene films found by Plyer and Peters (1950) and air in the vicinity of 6μ . The transmission curves for the KBr and KCl crystals with the various impurities investigated are shown in Fig. 1.

The position of the bands showing change under irradiation by ultraviolet are marked by arrows. As may be seen,

crystals with KNO_3 and KNO_2 impurities have no bands in the region under investigation other than those sensitive ultraviolet radiation.

Crystals with other impurities have, besides bands sensitive to the action of ultraviolet, a number of bands which do not show such sensitivity. No bands which undergo change during irradiation were found for crystals with impurities of K_2SO_4 , $\text{Na}_2\text{S}_2\text{O}_3$, NaSO_3 . In addition to the transmission measurements for crystals with impurities, the transmission of pure KBr crystals with a surface layer produced by placing the KBr monocrystal in an atmosphere of nitrogen oxides was also investigated. The layer obtained in this manner also had absorption bands at 7μ showing a sensitivity to ultraviolet radiation and to thermal treatment.

II. Changes in Absorption Connected with Thermal Treatment

1. KJ crystals¹

a) Changes in absorption with rapid cooling.

The absorption by KJ crystals before thermal treatment is shown in Fig. 2a. The arrows indicate the position of the bands sensitive to ultraviolet radiation. Fig. 2b shows the absorption of the same crystal after heating nearly to the melting point and followed by very rapid cooling. The crystal, after being heated in oven to the high temperature, was quickly removed from the oven and cooled in air for several minutes. The average cooling rate was of the order of 100°C per minute. As may be seen, the band next to the one sensitive to ultraviolet radiation becomes noticeably diffuse when the crystal is cooled rapidly. If the crystal is again heated and cooled slowly, the absorption returns to its initial shape.

b) Changes in absorption with an increase in temperature.

Transmission measurements were made for KJ crystals at different temperatures. The crystal being investigated was heated by means of a special Raman illuminator in which a heating coil wound on a ceramic rod replaced the mercury lamp.

All measurements were made in a state of thermal equilibrium i.e. when a thermocouple indicated a constant temperature. It was possible to chan-

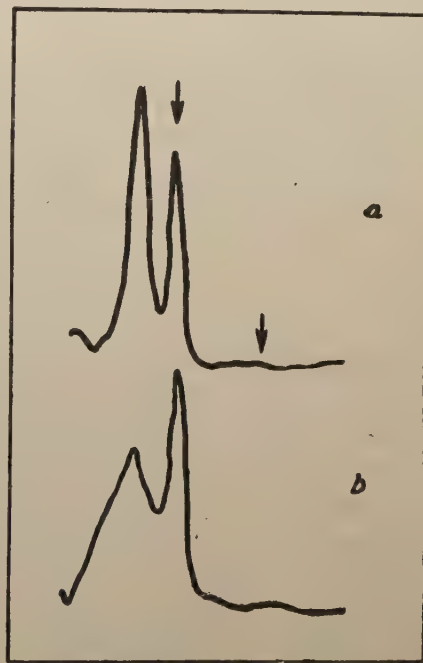


Fig. 2

¹ The initial material already contained a small quantity of unidentified impurities, probably K_2CO_3 .

ge the temperature by changing the heating current. The results are shown in Fig. 3.

As may be seen, the transmission increases with temperature, the absorption maximum shifting somewhat in the direction of the longer wavelengths. A closer analysis shows, however, that the increase in transmission observed above is only apparent.

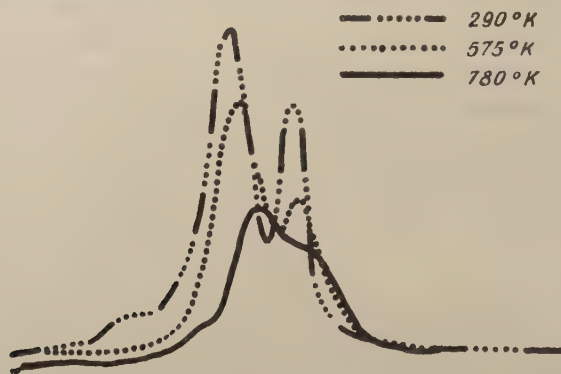


Fig. 3

It so happens that the crystal heated to a high temperature begins to emit radiation of the same wavelengths previously absorbed by it. This emission by the crystal produces the apparent increase in transmission.

Let us assume that the intensity of radiation emitted by a crystal at a given wavelength may be expressed as follows:²

$$\mathcal{E}_T = A \frac{\nu^3}{e^{\frac{h\nu}{kT}} - 1}$$

The crystal transmission at a given temperature for a given wavelength is $P_T = I'/I_0$, where $I' = I + I_1$. I' is the intensity of radiation reaching the detector and recorded by it. I is the intensity of the light passing through the crystal from the source, and I_1 is the intensity of the radiation emitted at the given temperature by the crystal in accordance with the above law. Therefore

$$P_T = \frac{I + I_1}{I_0} = P_0 + \mathcal{E}_T$$

where $P_0 = I/I_0$ and $\mathcal{E}_T = I_1/I_0$

Hence, for a given wave length,

$$P_T = P_0 + \frac{A}{e^{\frac{h\nu}{kT}} - 1}$$

² This approach is due to Professor A. Jabłoński to whom I wish to express my sincere gratitude.

$$\text{if } h\nu > kT \quad P_T = P_0 + Ae^{-\frac{h\nu}{kT}} \quad P_T - P_0 = Ae^{-\frac{h\nu}{kT}}$$

Denoting $h\nu = \Delta E$ we finally obtain

$$\lg(P_T - P_0) = \lg A - \frac{\Delta E}{2.3k} \frac{1}{T}$$

If we plot $\lg(P_T - P_0)$ as a function of $1/T$ we should obtain a line, and ΔE obtained from the slope of this line should equal ΔE calculated from the wavelength at which absorption takes place.

Fig. 4 shows the plot of $\lg(P_T - P_0)$ as a function of $1/T$. As may be seen, we obtain a line and we find that ΔE calculated from the slope of the line and from the wavelength at which we recorded absorption are in agreement within the limits of error of the measurement.

ΔE from the slope of the line — 0.173 eV

ΔE from the absorption wavelength — 0.179 eV

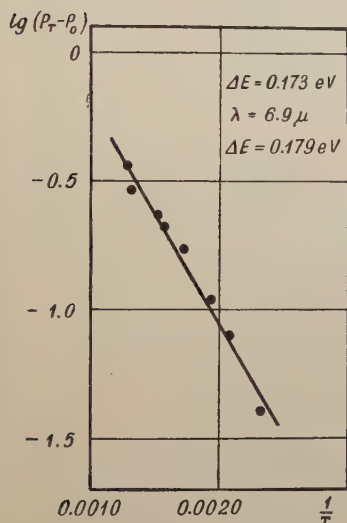


Fig. 4

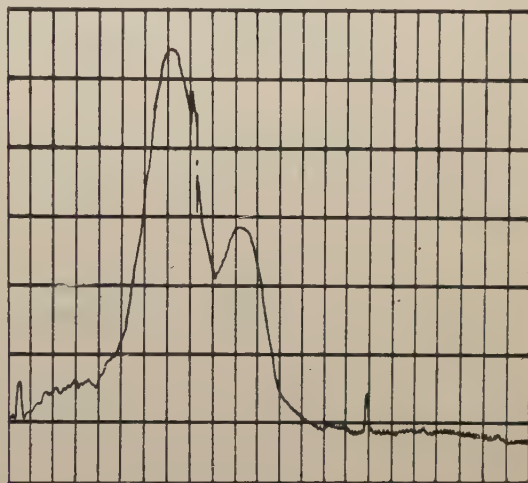


Fig. 5

It should be noted that this result also indicates that changes in temperature of the thermocouple situated in the direct vicinity of the crystal satisfactorily reflect the changes in the temperature of the crystal itself.

c) Changes in absorption by KJ crystals with simultaneous heating and irradiation by ultraviolet.

In these measurements the same equipment was used as in the investigation of changes in absorption with heating, except that a mercury lamp was placed in the illuminator instead of a heater.

The absorption by KJ crystals before irradiation is shown in Fig. 5. Fig. 6 shows the absorption in the KJ monocrystals after irradiation by ultraviolet. Fig. 7 shows the

absorption for the same monocrystals after lengthy illumination by ultraviolet and simultaneous heating. This heating could not be eliminated during the long period of irradiation, since the mercury lamp also emits a rich infrared spectrum.

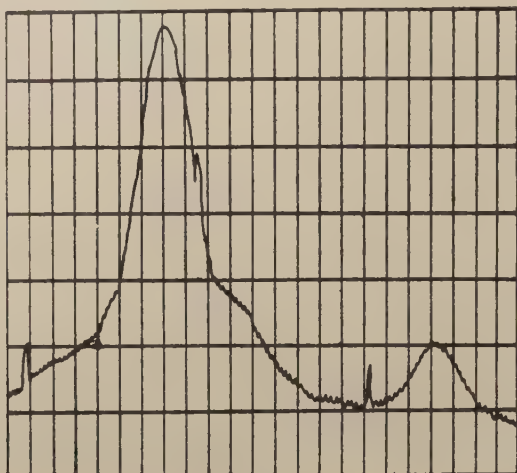


Fig. 6

The absorption obtained as a result of irradiation and heating is steady and does not change with time. Changes of absorption during simultaneous heating and ultraviolet irradiation were investigated for crystals already having an absorption as shown

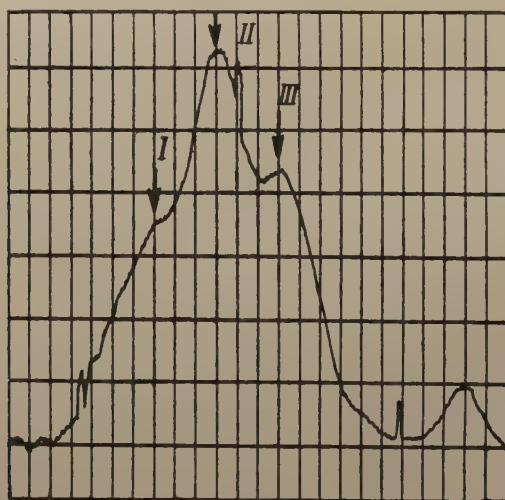


Fig. 7

in Fig. 7, these changes occurring for a wavelength corresponding to the position in the absorption band of wavelength indicated in Fig. 7 — I, II, III. The results of these measurements are shown in Fig. 8.

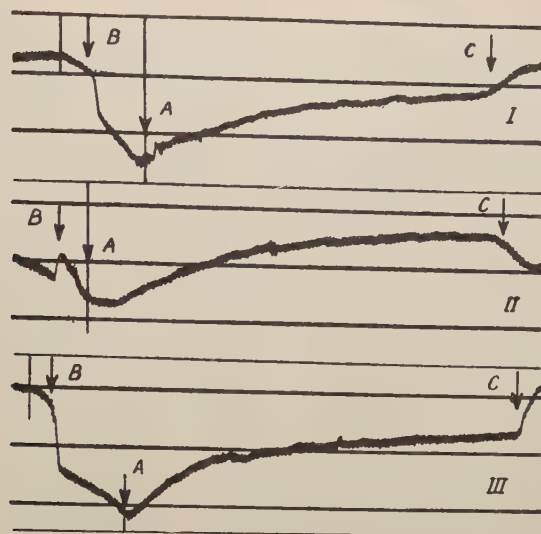


Fig. 8

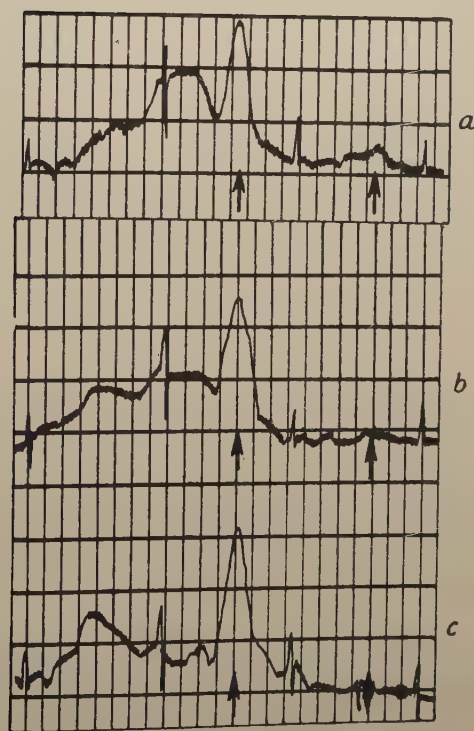


Fig. 9

The curves represent changes in absorption with time, during illumination and heating, for wavelengths corresponding to positions I, II, III in the absorption band. The crystal was irradiated and heated for a time indicated on the curves by *A*. At time *A* the mercury lamp was extinguished and the crystal was slowly cooled. The slow changes in absorption during heating should be associated with the apparent change in transmission resulting from emission by the crystal during heating. On the other hand, the sudden jump in absorption at *B* and *C* indicates some kind of internal changes taking place in the crystal at a certain temperature. Perhaps these changes are related to changes in structure occurring in the centres at a temperature correspond-

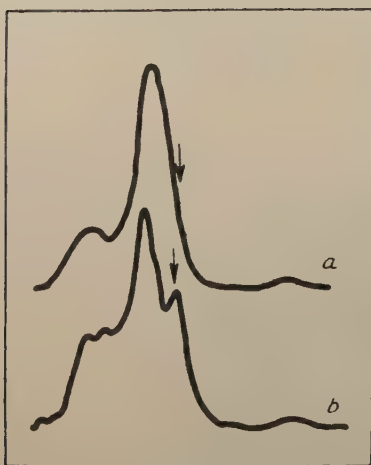


Fig. 10

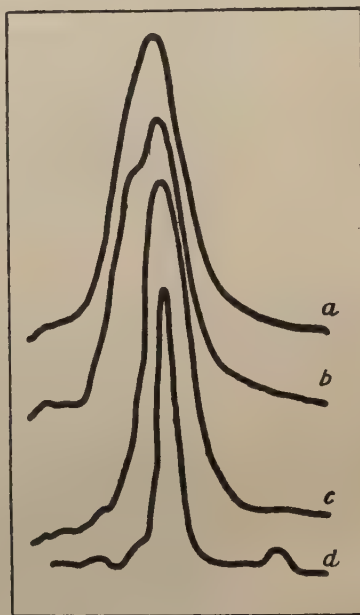


Fig. 11

ing to points *B* and *C*. For absorption in the infrared these changes, as may be seen from the curves, are indicated by the appearance or disappearance of the bands giving secondary maxima; at the same time changes also take place in the absorption in the central band. The explanation of the mechanism of these changes requires further detailed investigation. Such investigations were not made in the present work.

2. Changes in absorption associated with thermal treatment of other crystals.

Changes in absorption for KBr crystals with impurities of K_2CO_3 produced by more or less sudden cooling are shown in Fig. 9. Fig. 9a represents the absorption before the heat treatment of the crystal. Fig. 9b indicates the absorption after heating to a temperature of about $650^\circ C$ and with slow cooling. Fig. 9c shows the absorption

of the crystal after heating to a temperature of about 650°C followed by very rapid cooling. The arrows indicate the position of the band sensitive to ultraviolet radiation. Similar changes are also observed with heating followed by rapid cooling in the case of KBr monocrystals with a KOH impurity. Changes in absorption accompanying thermal treatment of such crystals are shown in Fig. 10.

(Note: In the case of activation by KOH the crystals may contain some amount of K_2CO_3).

Somewhat more attention was paid to the absorption of KBr monocrystals having a surface layer formed after placing these monocrystals in an atmosphere of nitrogen oxides. The existence of the above-mentioned layer is readily verified by viewing the monocrystal surface under polarized light. Fig. 11 (curve *a*) shows the absorption of a KBr monocrystal with such a layer. A characteristic feature of the absorption of the layer is a marked asymmetry and a large absorption band width. Also characteristic are changes of absorption with heating. The changes are illustrated, in turn, by curves *b*, *c*, and *d*. Curve *b* represents the absorption of the KBr crystal with a layer formed in nitrogen oxides after the crystal was heated to a temperature of 250°C and cooled to room temperature. Curve *c* represents the absorption of the KBr crystal with the layer after having been heated to 370°C and cooled to room temperature; finally curve *d* represents the absorption of the crystal heated to a temperature of 540°C and then cooled to room temperature. Curve *d* is analogous to that characterizing the absorption of KBr monocrystals with KNO_3 or KNO_2 impurities, except that the monocrystal having the layer and heated to a temperature of 540°C has only one distinct absorption maximum in the shorter wavelengths, while the monocrystal with the KNO_3 or KNO_2 impurities has two absorption maxima. For crystals with the layer the second maximum is barely visible and increases only after the heating to temperatures above 540°C. All changes of absorption with heating discussed above for monocrystals with a layer formed in nitrogen oxides are permanent and irreversible, in contrast to the changes observed for KJ crystals and KBr crystals with K_2CO_3 and KOH impurities.

III. Changes of Absorption With Irradiation in Ultraviolet

Besides the changes in absorption previously found by Wardzyński (1955) for irradiation of KBr monocrystals with KNO_3 , K_2CO_3 and KOH impurities, analogous changes were found for KBr monocrystals with KNO_2 impurities, KCl monocrystals with KOH impurities, and KBr monocrystals with a layer formed in an atmosphere of nitrogen oxides.

The investigated monocrystals were irradiated by the full light of a mercury lamp using the previously mentioned illuminator. The mercury lamp burner was situated at one focus of the elliptical mirror of the illuminator, the crystal being at the second focus. Fig. 12 shows a photograph of the illuminator employed.

Using a Wood filter and a filter from ordinary glass, it was shown that changes of absorption are due to the absorption of ultraviolet light of wavelength shorter than that passing through the Wood filter. The monocrystals have absorption bands in the ultraviolet at 2000–2200 Å. It should be supposed that the ultraviolet light absorbed precisely in these bands leads to the observed changes in absorption in the infrared. The changes of absorption in the infrared produced by irradiation of the KBr mono-



Fig. 12

crystal with a KNO_2 impurity is shown in Fig. 13. Curve *a* refers to the absorption before irradiation, curve *b* to the absorption after irradiation by ultraviolet. The absorption of KBr monocrystals with KNO_3 and KNO_2 impurities differs only in the ratio of the transmission in the band of shorter wavelength to that for the band of longer wavelength. The irradiation of KBr monocrystals with a KNO_3 impurity as well as those with a KNO_2 impurity leads to the gradual disappearance of the band of shorter wavelength, the band of longer wavelength increasing in intensity at the same time.

The absorption in infrared of KCl monocrystals with a KOH impurity consists of a number of bands, among which are also bands subject to changes during irradiation by ultraviolet. Curve *a* of Fig. 14 shows the absorption of such a crystal before irradiation and curve *b*, the absorption after irradiation. The arrows indicate the bands

undergoing changes in the case of irradiation. Here too, the band of shorter wavelength slowly disappears as the irradiation continues, while the band of longer wavelength gradually increases in intensity.

As we have already shown, the placing of the KBr crystal in an atmosphere of nitrogen oxides leads to the formation on the crystal surface of a layer absorbing the infrared of the same wavelengths as KBr monocrystals with KNO_2 or KNO_3 impurities, except that instead of two bands, we have only a clearly asymmetric and rather diffuse band in the shorter wavelengths. It was established that the irradiation of such a layer in ultraviolet results in the appearance of the previously absent band of longer wavelength, the wavelength being the same as in the case of KBr with KNO_3 or KNO_2 impurities. Curve *a* of Fig. 15 shows the absorption of such a layer before irradiation. Curve *b* shows the absorption of this layer after 10 min. of irradiation. Finally, curve *c* shows the absorption after 60 min. of irradiation by the full light of the mercury lamp.

We have also shown that the absorption of such a layer undergoes change when heated to a temperature of several hundred degrees C. The absorption band becomes considerably sharper, and the absorption maximum increases. The absorption band of such a layer, after heating, does not differ in shape or position from the absorption bands observed in KBr monocrystals with KNO_3 and KNO_2 impurities.

Fig. 16 shows the changes in such absorption bands arising during ultraviolet irradiation. Curve *a* shows the absorption before irradiation, curve *b* — after 4 min. of irradiation and curve *c* — after 19 min. of irradiation. Note should be taken of the

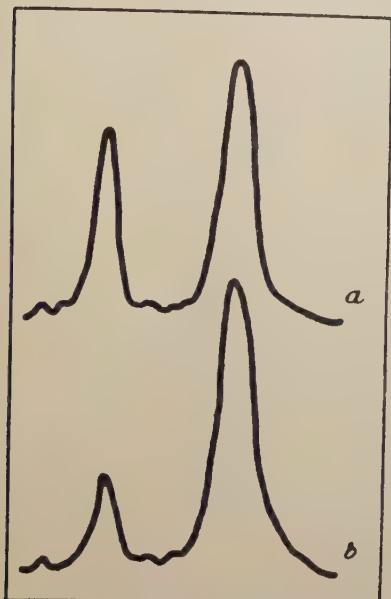


Fig. 13

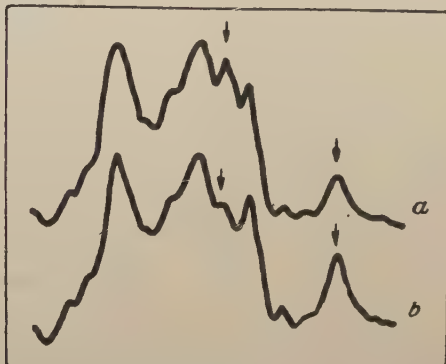


Fig. 14

fact that it is considerably easier to produce in the heated layer changes of absorption by irradiation than in the previous cases. In connection with the observed changes in absorption with ultraviolet radiation, there comes to the fore the question of whether the disappearance of one of the bands and the increase in intensity of the other are connected with the same process taking place in the centres responsible for absorption, or whether these are two different processes. At the same time, the gradual disappearance of one band and the increase of the intensity of the second suggest that the changes in these bands are connected with one another. Figs. 17 and 18 show how shape of the bands of shorter (Fig. 17) and longer (Fig. 18) wavelength change during irradiation. Comparison of Fig. 17 and Fig. 18 might give rise to doubts as to the precise connection between both bands. The above problem might be solved by establishing how the number of absorbing centres from one band decrease during irradiation and how the

number of centres associated with the second band increase at the same time. The product of the half-width of a given band and the absorption coefficient at the maximum of this band may serve as a measure of the number of absorbing centres associated with the band. If the reflection coefficient R is taken, in approximation, equal to zero, then the absorption coefficient will be proportional to the logarithm of the inverse of the transmission of the crystal. Measurements were made of the changes in the transmission and half-width of the absorption bands as a function of the irradiation time. During irradiation the crystal was always placed at the same distance from the mercury lamp burner so that the irradiation time was proportional to the amount of luminous energy reaching the crystal. The results of measurements of the KBr crystal with

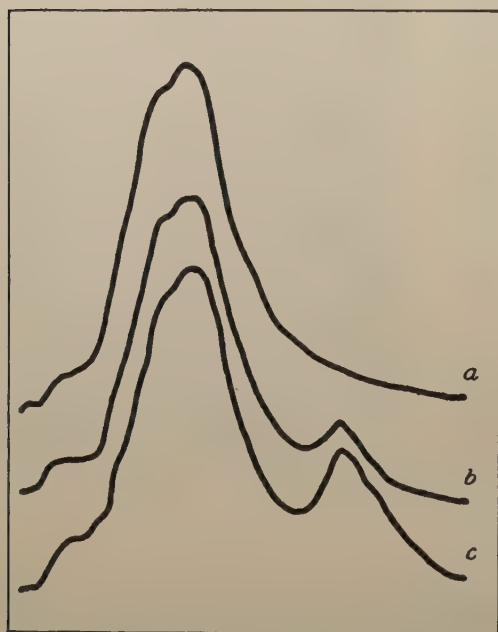


Fig. 15

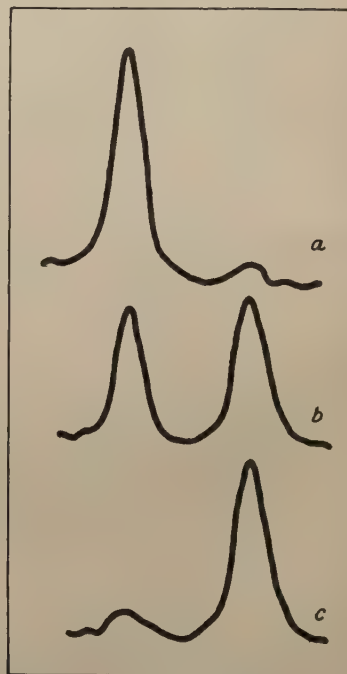


Fig. 16

a KNO_3 impurity are given by the curves in Fig. 19a, b, c. The solid curve (Fig. 19a) refers to the maximum of shorter wavelength and the dashed curve (Fig. 19b) to the maximum of longer wavelength. As may be seen from Fig. 19a, the number of absorbing centres associated with the band of longer wavelength changes within the limits of error of measurement according to the law

$$\frac{1}{N} = A + Bt$$

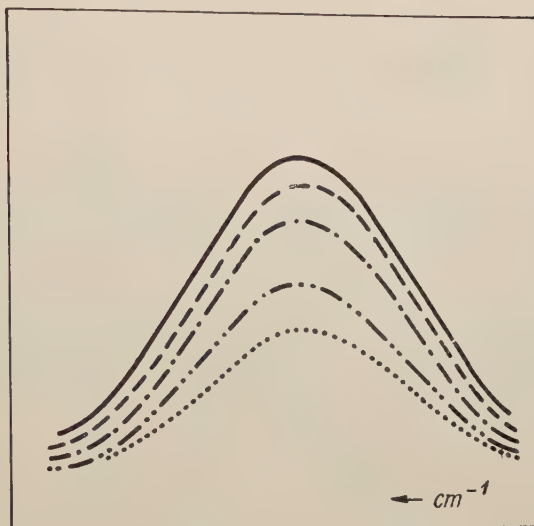


Fig. 17. Variation of absorption of the band at 7μ during irradiation of the KBr KON_3 crystal by ultraviolet

— before irradiation · · · · · after 34 min. of irradiation
 - - - - - after 3 min. of irradiation · · · · · after 64 min. of irradiation
 - · - · - after 9 min. of irradiation

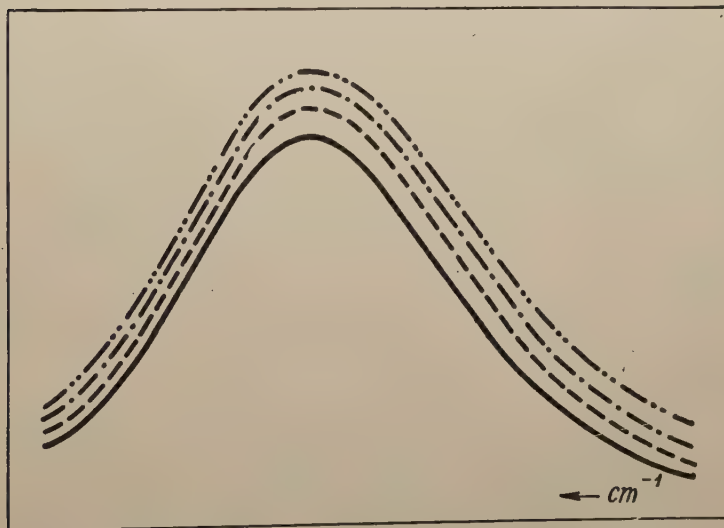


Fig. 18. Variation of absorption of the band at 8μ during irradiation of the KBr KNO_3 crystal by ultraviolet.

— before irradiation - · - · - after 9 min. of irradiation
 - - - - - after 3 min. of irradiation · · · · · after 34 min. of irradiation

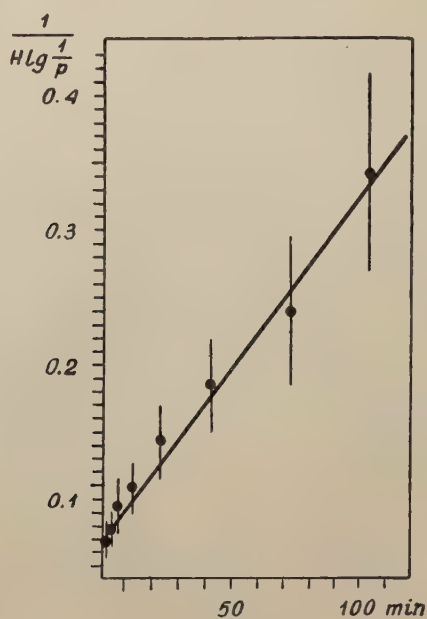


Fig. 19a

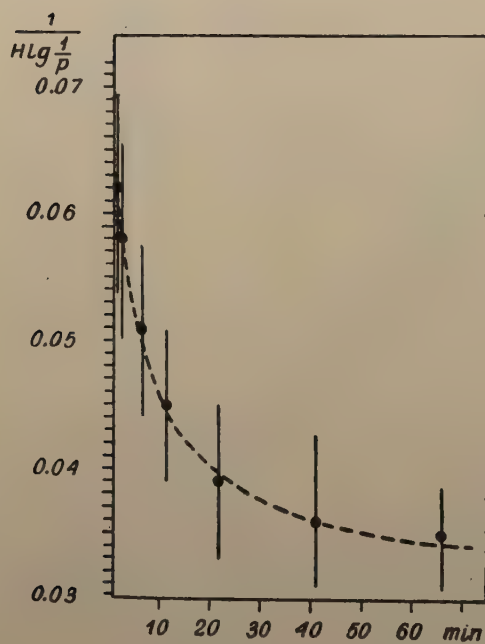


Fig. 19b

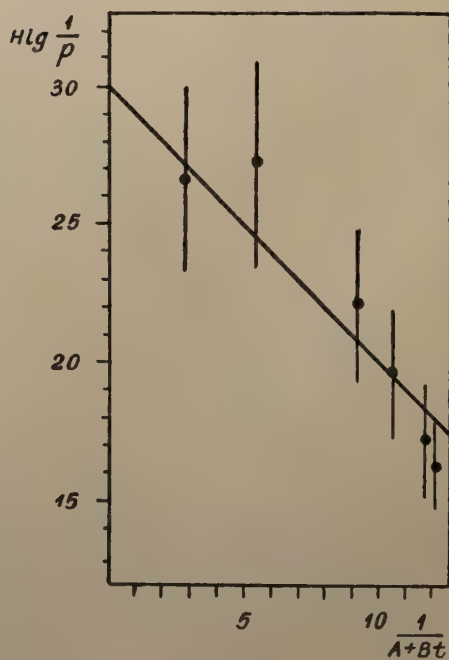


Fig. 19c

since the expression $(H \lg 1/P)^{-1}$ (where H is the half-width of the band and P is the transmission at the maximum absorption of the band) is proportional to $1/N$. After differentiation of this term, we obtain:

$$\frac{dN}{dt} = -BN^2$$

and therefore the rate at which the absorbing centres in the band of shorter wavelength decreases is proportional to the square of the number of centres existing at the given time. Let us assume that the total number of centres responsible for absorption in both bands does not change during irradiation. We denote the number of absorbing centres of the band of shorter wavelength by N_1 and the band of longer wavelength by N_2 . Let the total number of centres be $N = N_1 + N_2$. Taking into account that

$$\frac{1}{N_1} = A + Bt$$

we obtain, after simple transformation,

$$N_2 = N - \frac{1}{A + Bt}$$

From the curve in Fig. 19a we can determine A and B . ($A = 0.08$, $B = 0.0026$); then for the band of longer wavelength we can plot $H \lg 1/P$ as a function of $1/(A + Bt)$. Fig. 19c gives such a curve. As may be seen, the assumption that the total number of centres responsible for absorption in both bands does not change during irradiation is confirmed within the limits of experimental error. Since, as we have already shown, $(H \lg 1/P)_I$ is proportional to N_1 and $(H \lg 1/P)_{II}$ is proportional to N_2 , then the sum $(H \lg 1/P)_I + (H \lg 1/P)_{II}$ should not change. The subscript I refers to the band of shorter wavelength band, while the subscript II refers to the band of longer wavelength. The term $H \lg 1/P$ will be proportional to N only if the reflection coefficient can be taken as zero. The reflection coefficient is, however, not equal to zero and changes with the change in transmission during irradiation; the value of $(H \lg 1/P)_I + (H \lg 1/P)_{II}$ determined on the basis of the measurements will contain some error especially during the first period of irradiation. Table I gives the results of the measurements for a KBr crystal with a KNO_3 impurity.

Table I

Crystal	Irradiation minutes	$(H \lg 1/P)_I + (H \lg 1/P)_{II}$
KBr KNO_3	1	28.5 ± 4
	2	29.0 ± 4
	6	29.1 ± 4
	11	30.7 ± 4
	41	32.0 ± 4
	101	29.6 ± 4

If we consider that we have not taken the reflection coefficient into account, then the constancy of the sum $(H \lg 1/P)_I + (H \lg 1/P)_{II}$ should be regarded as sufficient. It may then be assumed that, within the limits of accuracy of the measurements, the sum of the centres responsible for absorption in both bands remains constant during irradiation.

IV. Relation Between the Coefficient of Absorption and the Number of Absorbing Centres. Shape of the Absorption Band

The relation between the coefficient of absorption and the number of absorbing centres may be found by using the Lorentz-Lorenz formula:

$$\frac{n^{*2} - 1}{n^{*2} + 2} = \frac{4}{3} \pi N \alpha$$

In this formula n^* is the coefficient of refraction, and α is polarizability. Since

$$\alpha = \frac{e^2}{m} \sum_{\nu} \frac{f_{\nu}}{(\omega^2 - \omega_{\nu}^2) + i\omega H}$$

we thus obtain the well-known dispersion formula:

$$\frac{n^{*2} - 1}{n^{*2} + 2} = \frac{1}{3} \sum_{\nu} \frac{a_{\nu} f_{\nu}}{(\omega^2 - \omega_{\nu}^2) + i\omega H}$$

In this formula

$$a_{\nu} = \frac{4\pi N e^2}{m}; \quad n^* = n_0 (1 - i\kappa); \quad \kappa = \frac{K\lambda_0}{4\pi n_0}$$

f_{ν} is the oscillator strength, N is the number of oscillators in a unit volume, e is the charge associated with the oscillator, m is the mass of the oscillator. This formula, which takes into account the damping of the vibrations, also gives the dispersion inside the absorption band. If we limit ourselves to only one absorption band, we obtain a relation representing the variation of the dispersion in the region of this band:

$$\frac{n^{*2} - 1}{n^{*2} + 2} = \frac{4\pi N e^2}{3m} f \frac{1}{\omega^2 - \omega_0^2 + i\omega H} \quad (1)$$

From this it is easy to find the sought-for relation between the coefficient of absorption and the number of absorbing centres, assuming, following Koch (1930) and Smakula (1930), that the change in the refraction coefficient caused by the introduction of the impurities is small ($n = n_0 + \Delta n$) and taking into account the fact that $\kappa = K\lambda_0/4\pi n_0$ is small. (In our case it is readily shown that κ is of the order 10^{-4} .) Since Δn and κ are small, we may neglect terms containing the product $\Delta n \kappa$ and higher powers of these quantities. Taking the imaginary part of (1), we obtain

$$\frac{\kappa n_0^2}{(n_0^2 + 2)^2} = \frac{2\pi N e^2}{9m} f \frac{H\omega}{(\omega_0^2 - \omega^2)^2 + H^2 \omega^2}$$

from which we have

$$K = \frac{2Ne^2f(n_0^2 + 2)^2}{mc^2 9n_0} \cdot \frac{H\nu^2}{(\nu_0^2 - \nu^2)^2 + H^2\nu^2}$$

In order to compare the obtained formula with experiment we note that

$$K = \frac{2.3}{d} \lg \frac{(1 - R)^2}{P}$$

Denoting

$$\frac{2Ne^2f(n_0^2 + 2)^2}{mc^2 9n_0} = A$$

we have

$$K = A \frac{H}{\left[\frac{\nu_0^2}{\nu} - \nu \right]^2 + H^2}$$

From this

$$\lg \frac{(1 - R)^2}{P} = \frac{d}{2.3} \frac{AH}{\left[\frac{\nu_0^2}{\nu} - \nu \right]^2 + H^2}$$

and finally

$$\frac{1}{\lg \frac{(1 - R)^2}{P}} = \frac{2.3 H}{dA} + \frac{2.3}{dAH} \left[\frac{\nu_0^2}{\nu} - \nu \right]^2$$

We denote

$$\frac{2.3 H}{dA} = \alpha \quad \text{and} \quad \frac{2.3}{dAH} = \beta$$

Then

$$\frac{1}{\lg \frac{(1 - R)^2}{P}} = \alpha + \beta \left(\frac{\nu_0^2}{\nu} - \nu \right)^2$$

In the case of $R = 0$ we will have

$$\frac{1}{\lg \frac{1}{P}} = \alpha_0 + \beta_0 \left(\frac{\nu_0^2}{\nu} - \nu \right)^2$$

where ν_0 is the frequency corresponding to the absorption maximum and α_0 and β_0 are certain constants. If a plot of $1/\lg 1/P$ vs the function $[(\nu_0^2/\nu) - \nu]^2$ is made,

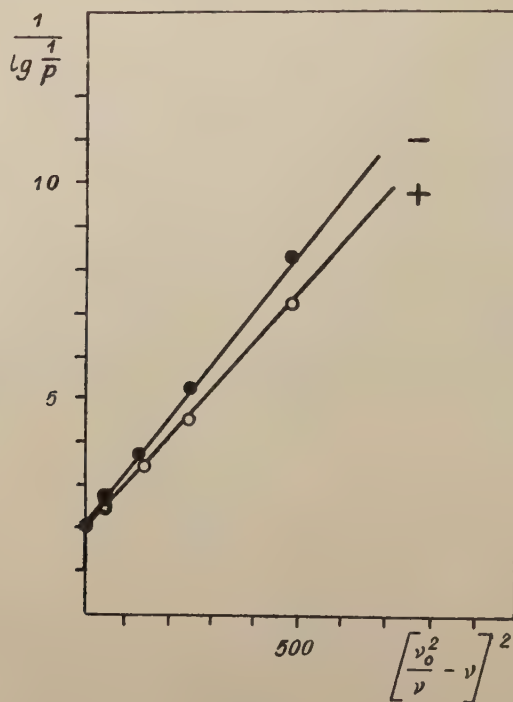


Fig. 20

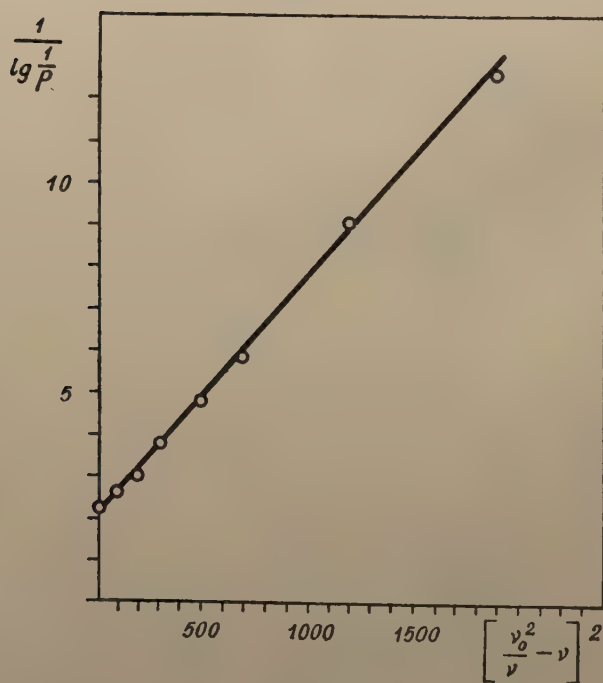


Fig. 21

then, if our considerations are correct, a straight line should be obtained. The corresponding curve for the crystal KBrKNO_3 No. 4 is given by Fig. 20. This curve refers to the maximum of shorter wavelength. Because of the asymmetry of the band, we obtain for the positive branch ($\nu > \nu_0$) a line of somewhat different slope than for the negative branch ($\nu < \nu_0$). As may be seen, both the positive and negative branches can be represented by the expression

$$\frac{1}{\lg 1/P} = \alpha_0 + \beta_0 \left[\frac{\nu_0^2}{\nu} - \nu \right]^2$$

In the case of the positive and negative branches, only β_0 will differ somewhat. Fig. 21 shows a similar curve for the band of longer wavelength.

V. Measurements of the Coefficients of Absorption and Reflection

1. Coefficients of absorption and reflection at the band maximum.

In order to find the absorption and reflection coefficients for a given crystal, transmission measurements should be made for slabs of this crystal of different thickness. Since $P = (1 - R)^2 e^{-Kd}$, then, laying off the transmission along one axis in a logarithmic scale, and the corresponding thickness of the crystal slab along the other, we obtain a line. The slope of the line determines the coefficient of absorption. For $d = 0$ we have $P = P_0 = (1 - R)^2$, from which we find R . The slab thickness was measured by means of microscope of low magnification. First focussing one, and then the other, surface of the slab, we measure the displacement of the microscope tube. If this displacement is d_1 then the thickness d of the crystal slab is $d = nd_1$, where n is the index of refraction for the light illuminating the slab. Thickness measurements were repeated at various points on the slab and the mean was taken. The results of the measurements for the maximum of shorter wavelength are given in Fig. 22. Fig. 23 gives the results of the measurements for various crystals in the case of the maximum at the longer wavelength. Table II lists the values of the absorption and reflection coefficients calculated on the basis of data from the curves in Figs. 22 and 23.

Table II

Crystal	Maximum at $\lambda = 7\mu$		Maximum at $\lambda = 8\mu$	
	K	R	K	R
KBrKNO ₃ No. 1	15.5 cm ⁻¹	0.35	18.9 cm ⁻¹	0.28
KBrKNO ₃ No. 2	7.5 cm ⁻¹	0.16	5.7 cm ⁻¹	0.03
KBrKNO ₃ No. 3	8.9 cm ⁻¹	0.22	7.2 cm ⁻¹	0.16
{ KBrKNO ₃ No. 4 irradiated by ultraviolet	4.0 cm ⁻¹	0.05	13.5 cm ⁻¹	0.14

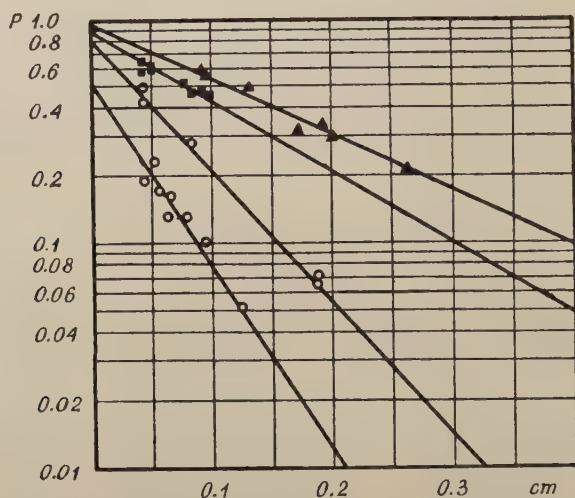


Fig. 22. Variation of transmission with crystal thickness for the band at 7μ .

- KBr KNO_3 crystal No. 1
- KBr KNO_3 " No. 4
- ▲ KBr KNO_3 " No. 3
- KBr KNO_3 " No. 4 irradiated by ultraviolet

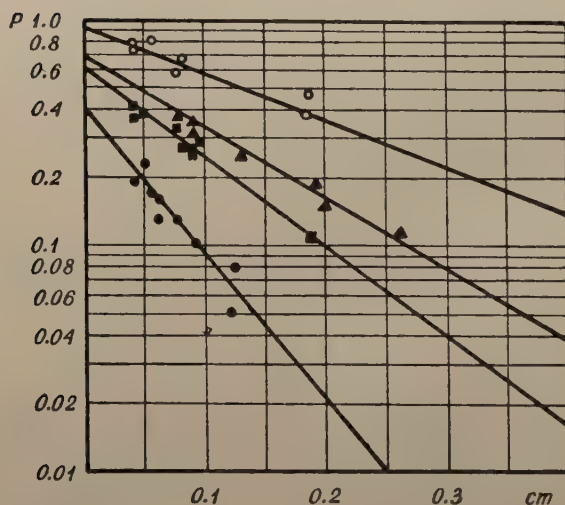


Fig. 23. Variation of transmission with crystal thickness for the band at 8μ .

- KBr KON_3 crystal No. 1
- KBr KNO_3 " No. 4
- ▲ KBr KNO_3 " No. 3
- KBr KNO_3 " No. 4 irradiated by ultraviolet

2. Changes in the coefficients of absorption and reflection inside the absorption band.

If, as in the case of measurements of the maximum coefficient of absorption, the transmission corresponding to different slab thicknesses and different points in the absorption band is laid off along one axis in a logarithmic scale, the coefficient of absorption at different points of the band and the coefficient of reflection at these

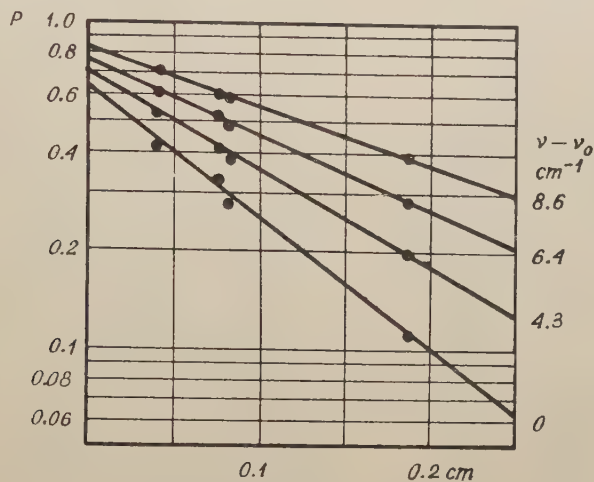


Fig. 24

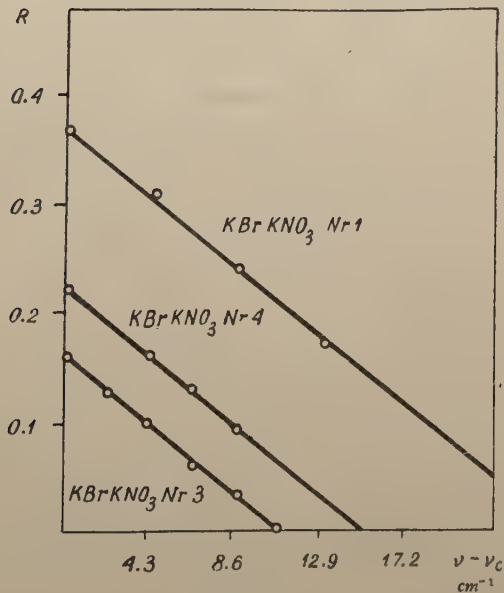


Fig. 25

points can be determined. Such curves for the KBrKNO_3 crystal No. 4 are shown in Fig. 24. The values of R found for different crystals are shown on the curve of Fig. 25.

As may be seen from the curves, the coefficient of decreases approximately linearly with an increase in $\nu - \nu_0$, the changes for different crystals having the same character. The coefficient R at any point of the absorption band can be determined from the approximate empirical formula derived on the basis of the curves in Fig. 25.

$$R = R_0 - 0.015 |\Delta\nu|$$

where R_0 is the highest coefficient of reflection at the point $\nu = \nu_0$ of the band, and $|\Delta\nu| = |\nu - \nu_0|$.

The variation of K with $\nu - \nu_0$ can also be determined from Fig. 24; this means that the absorption band can be found in a scale of absorption coefficients, and not as thus far, in a scale of transmission. Fig. 26 gives a plot of K vs $\nu - \nu_0$ for the KBrKNO_3 crystal No. 4. From this last curve the value of the half-width of the absorption band can be found. We note that the half-width can also be found independently if we plot

$$\frac{1}{\lg \frac{(1-R)^2}{P}} = \alpha + \beta \left(\frac{\nu_0^2}{\nu} - \nu \right)^2$$

We can plot this relation if we know how R varies inside the absorption band. Since

$$\alpha = \frac{2.3 H}{dA} \text{ and } \beta = \frac{2.3}{dAH}$$

then

$$\frac{\alpha}{\beta} = H^2$$

H determined in this way is in good agreement with that found from direct measurements.

VI. Variation of Absorption With Temperature

1. Equipment.

Measurements were made of transmission both at a temperature lower than room temperature and at higher temperatures. At temperatures higher than room temperature it was checked whether the crystal emits energy in the region in which the mea-

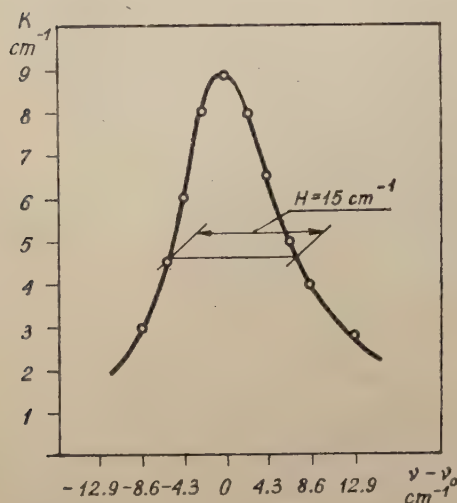


Fig. 26

measurements were made and whether the observed changes in transmission are not caused by the emission of radiation as in the case of KJ crystals. A series of measurements was also made on a single-beam Marconi spectrometer having a modulated light source, owing to which any radiation of the sample was eliminated. Changes in absorption with temperature, recorded by means of the Hilger and Marconi spectrometers, proved to be identical. In the case of the Marconi spectrometer the spectrum was observed on the screen of an oscilloscope tube and recorded by photographing the screen. In addition, in order to accentuate the effect of the emission of radiation on the observed transmission of the crystals, the temperature was limited to somewhat lower temperature than in the case of KJ crystals. Both the heating and the cooling of the crystals took place somewhat differently from the case of measurements of the change in transmission for KJ crystals. The crystals were not placed, as before, at the focus of the elliptical mirror of the illuminator, but in a special vessel containing a sodium chloride window from which it was possible to remove the air. The crystal temperature was measured by means of a thermocouple introduced into the vessel and in direct contact with the crystal. The construction of the vessel is shown in Fig. 27.

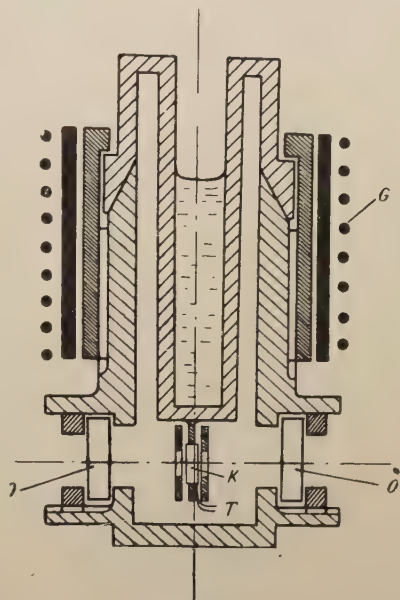


Fig. 27

On this drawing *O* denotes the NaCl window, *T* the thermocouple, *K* the crystal, *G* the heating coil wound on a layer of asbestos. The crystal was cooled by means of liquid air, solid carbon dioxide, and a mixture of carbon dioxide and alcohol. Heating coil *G* served to prevent condensation of water on window *O*. In addition, by changing the heating current and the level of the liquid in the vessel, it was possible to change the temperature of the crystal.

In the case of temperatures higher than room temperature, instead of liquid air, a heater wound on a ceramic tube was placed inside the vessel. All measurements were made at a constant temperature, in a state of thermal equilibrium. The evacuation of air from the vessel in the case of lower temperatures is necessary in order to prevent the formation of a layer of ice and solid CO_2 on the surface of the crystal.

2. Variation of the absorption band half-width with temperature.

As we have already shown, it is possible to determine the half-width of the absorption band from the dependence of $1/\lg [(1 - P)^2/P]$ on $[(\nu_0^2/\nu) - \nu]^2$. Fig. 28 is a plot of the above dependence for different temperatures of the KBrKNO_3 crystal No. 4. The curves are for the band of shorter wavelength under the assumption that $R = 0$.

Since $\alpha_0/\beta_0 = H_0^2$, then knowledge of α_0 and β_0 at different temperatures allows us to find the variation of H_0 with temperature. (The subscript "o" denotes that the given quantity refers to the case in which we neglect the coefficient of reflection R). Fig. 29 is a plot of the half-width of the absorption band of shorter wavelength as a function of temperature. H_0 was determined from the ratio α_0/β_0 , H_p was determined on the basis of direct measurements of the half-width of the absorption band in a scale of transmission. $H(T)$ was drawn as a curve lying between the curves of $H_0(T)$ and $H_p(T)$. $H(T)$ gives the true value of the half-width of the absorption band which

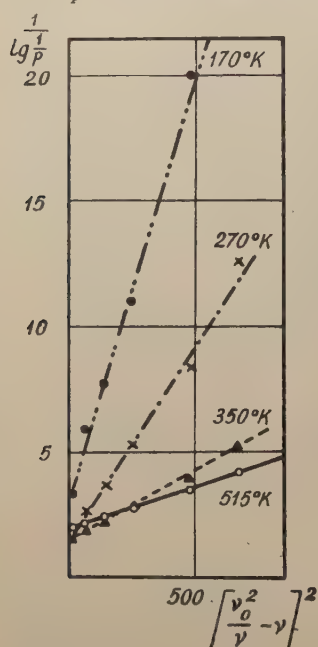


Fig. 28

we should obtain after taking into account the coefficient of reflection R . Proceeding in a similar way, we also determined the variation of the half-width of the absorption band of longer wavelength with changes in temperature. Plots of $H_0(T)$ and $H_p(T)$ are given in Fig. 30.

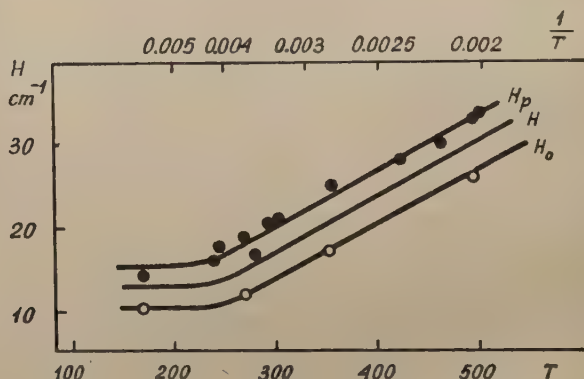


Fig. 29

As may be seen from the curves, H_0 and H_p differ very little. This is because the coefficient of reflection for this band is very small and may be neglected at least for higher temperatures.

3. Variation of transmission with temperature.

The transmission of a KBrKNO_3 crystal at various temperatures is given in Fig. 31. The different behaviour of the bands of shorter and longer wavelength stands out plainly.

In the second band, the transmission increases with an increase in temperature; at the same time the half-width also increases. The absorption maximum shifts somewhat towards the longer waves. The area under the curves seems to remain constant at different temperatures. The behaviour of the first band is completely different. The transmission at first decreases with an increase in temperature, it attains a mini-

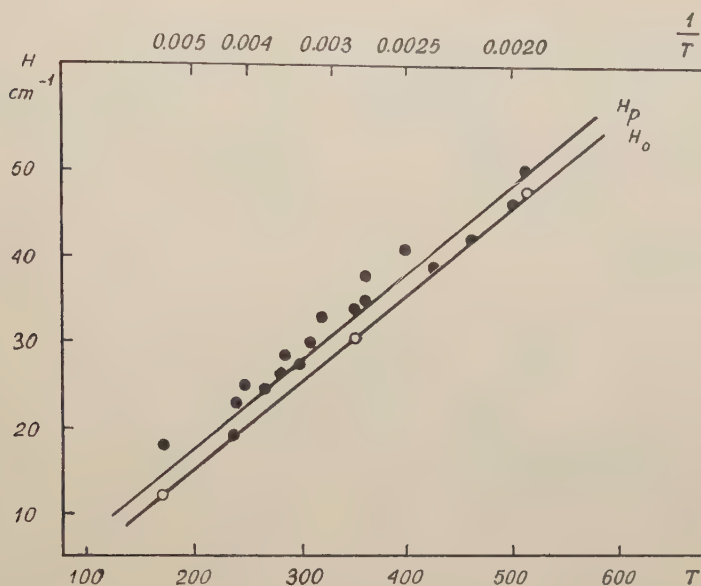


Fig. 30

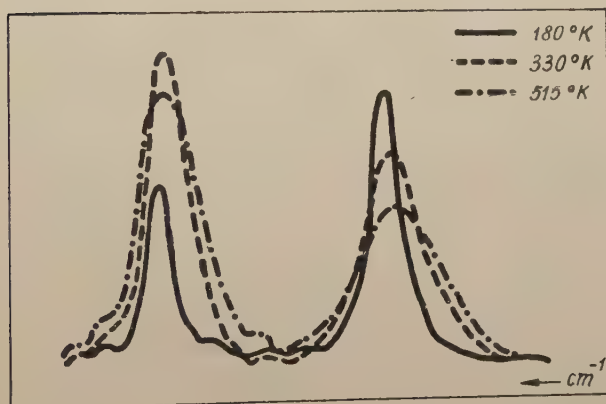


Fig. 31

mum and only then increases like the other band. The half-width for this band also increases with an increase in temperature, so that the area under the curve in the low-temperature region distinctly increases. A more detailed investigation was made of the changes of transmission as a function of temperature. These measurements also permitted us to find the variation of the coefficient of reflection with temperature. It turned out that the variation of R with temperature has the same character as the variation of the coefficient of absorption with temperature.

4. Variation of the number of absorbing centres with temperature.

If we take $R = 0$, then $\lg 1/P$ is proportional to the coefficient of absorption. The assumption $R = 0$, however, is not completely justified. Since we know how R varies with temperature, we can plot $\lg [(1 - R)^2/P]$ as a function of $1/T$, which illustrates the corresponding variation of the coefficient of absorption.

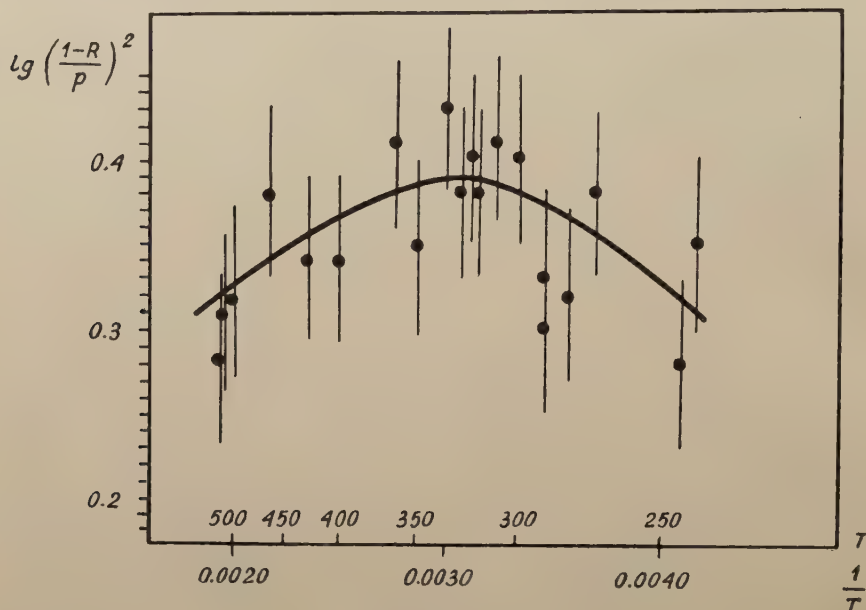


Fig. 32

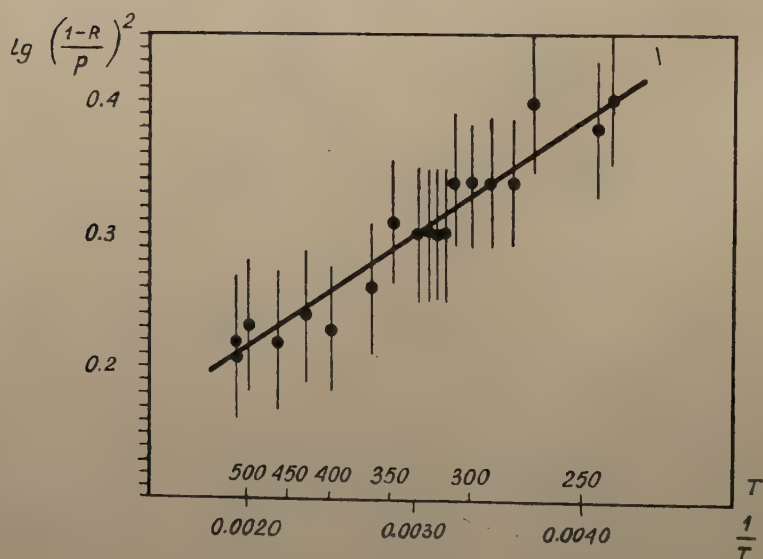


Fig. 33

Fig. 32 contains such a curve for the band of shorter wavelength for the KBrKNO₃ crystal No. 4. Fig. 33 gives the curve for the band of longer wavelength.

As we have seen, the number of absorbing centres is connected with the coefficient of absorption by the following expression:

$$K = \frac{2Ne^2 f(n_0^2 + 2)^2}{mc 9n_0} \cdot \frac{H\nu^2}{(\nu_0^2 - \nu^2)^2 + H^2 \nu^2}$$

If the coefficient of absorption is measured at the maximum of the absorption band, then for $\nu = \nu_0$ we then have

$$K_{\max} = \frac{2Ne^2 (n_0^2 + 2)^2 f}{mc 9 n_0} \cdot \frac{1}{H}$$

of $K_{\max} = A_1 N/H$, where A_1 is some constant. Since K_{\max} is proportional to $\lg [(1 - R)^2/P_{\min}]$, then $N \sim H \lg [(1 - R)^2/P_{\min}]$. Fig. 34 shows a plot of $\lg (H \lg (1 - R)^2/P_{\min})$ as a function of $1/T$ for the shorter wave maximum of the KBrKNO₃ crystal No. 4.

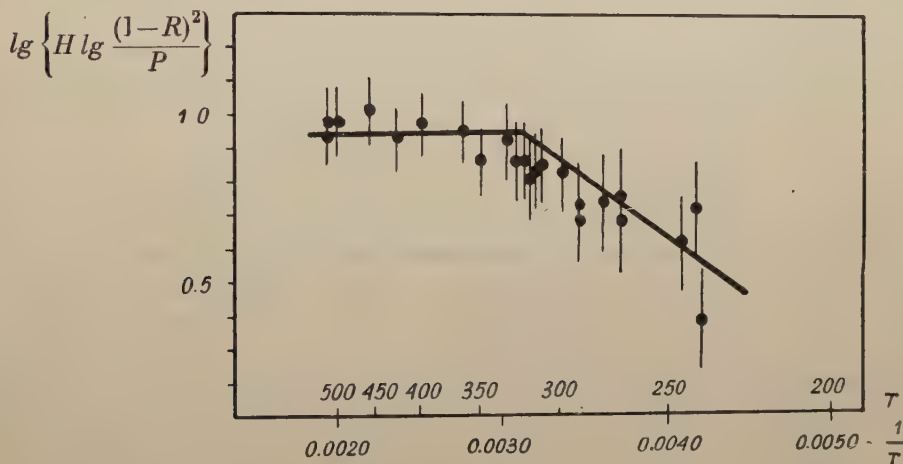


Fig. 34

We see that the quantity $H [\lg (1 - R)^2/P_{\min}]$, proportional to the number of centres N , is constant at high temperatures up to about 300°K, and then decreases. Whereas the character of this variation is entirely certain, the precise determination of the law according to which the number of centres decrease is difficult because of the large errors of measurement. It seems that $\lg N$ varies linearly with the inverse of the temperature. Therefore N would vary according to the law

$$N = N_0 e^{-\frac{B_1}{T}}$$

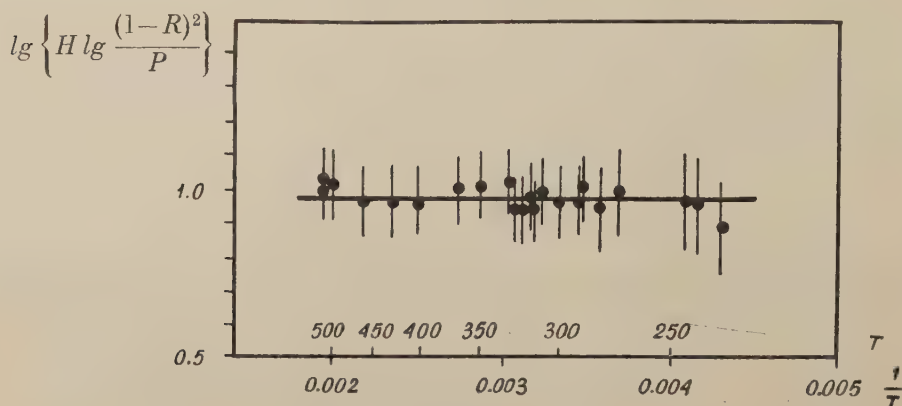


Fig. 35

An accurate confirmation of this relation requires further more precise measurements. Fig. 35 gives the analogous curve for the band of longer wavelength. From the curve it follows that, within the limits of error, the number of centres responsible for absorption in this band does not change with temperature in the temperature region investigated.

VII. Relation Between Absorption and the NO_2^- and NO_3^- Ion Concentration in Crystals With KNO_3 impurities

The concentration of NO_2^- and NO_3^- ions in the crystals under investigation can be determined by polarographic measurements. Such measurements were made by Z. Grabowski at the Institute of Chemistry of Warsaw University. The polarographic analysis disclosed the presence of NO_2^- and NO_3^- ions in the crystals to which KNO_3 was added. The total concentration of NO_2^- and NO_3^- ions resulting from the polarographic measurements is about three times smaller than the concentration of NO_3^- ions calculated from the quantity of KNO_3 added during production. The analysis showed that crystals with K_2CO_3 and KOH impurities do not contain either NO_3^- or NO_2^- ions, as should have expected. During the polarographic measurements, however, it was established that two waves of unknown origin indicate the possible presence of an unidentified impurity. Attention is drawn by the fact that the KBrKNO_3 crystals irradiated with ultraviolet show, during the polarographic measurements, a non-typical wave associated with the NO_3^- ion. The polarographic measurements made for different crystal samples from the same cluster show a somewhat different NO_3^- and NO_2^- ion content, the sum of the concentration of both ions, however, remains constant within the limits of error of the measurement.

Crystals irradiated by ultraviolet have, as shown by the polarographic measurements, a considerably smaller concentration of NO_3^- and considerably greater concentration of NO_2^- than before irradiation. The sum of the concentrations before and after irradiation did not change. If the crystal irradiated by ultraviolet is heated to

a high temperature and cooled, and then the polarographic measurements are made, it turns out that the NO_2^- and NO_3^- ion content does not differ, within the limits of error of the measurements, from the ion content in the crystal before irradiation. In other words, changes in the ion concentration produced by irradiation are irreversible after the crystal has been heated to a temperature of about 650°C , just as in the case of changes observed in the absorption in the infrared.

It was already pointed out above that there is a relation between the coefficient of absorption, half-width of the absorption band, and the number of oscillator centres responsible for absorption. Since K_{max} and H can be obtained from the infrared measurements, then, if we can calculate for our case the constant A_1 , we shall be able to calculate, on the basis of the absorption data, the number of centres according to the formula

$$K_{\text{max}} = A_1 \frac{N}{H}$$

It is interesting to compare the numbers obtained from the infrared measurements with the polarographic measurements. If we associate the band of shorter wavelength with the NO_3^- ions and the band of longer wavelength with the NO_2^- ions, and if we lay off along one axis the product $K_{\text{max}} \cdot H$ for the band of shorter wavelength, and along the other axis the corresponding concentration of NO_3^- ions determined by the polarographic method (points denoted by triangles), and the product $K_{\text{max}} \cdot H$ for the band of longer wavelength vs the concentration of NO_2^- ions (points denoted by circles), then, as shown by Fig. 36, we obtain, within the limits of experimental error, a straight line passing through the origin of the coordinate system, and on which lie both types of points.

Hence the number of absorption centres (proportional to $K_{\text{max}} H$) in each band is proportional to the respective concentration of the NO_3^- and NO_2^- ions, the coefficient of proportionality being the same for both types of ions and for both bands. If we measure K_{max} and H in cm^{-1} , then

$$N = A \cdot K_{\text{max}} \cdot H$$

where

$$A = \frac{c^2 m n_0}{2e^2 (n_0^2 + 2)^2}$$

If we substitute the values $c = 2.998 \times 10^{10}$ cm/sec and $n_0 = 1.53$ from the measurements of Gunderlach (1930), and if we take for NO_3^- (vibrations between oxygen and

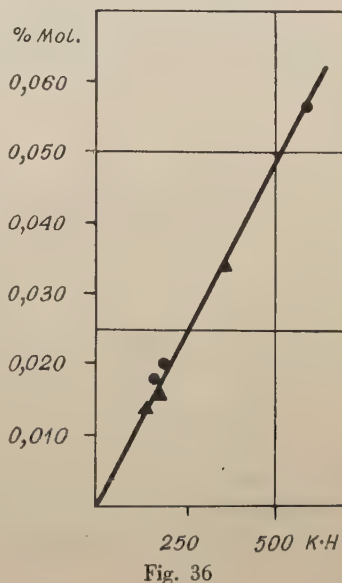


Fig. 36

nitrogen) the reduced mass of oxygen and nitrogen to be equal to 1.24×10^{-23} g and the charge of one N — O oscillation equal to $2/3 e$, where $e = 4.8 \times 10^{-10}$ cm dyne $^{1/2}$, we obtain

$$A = 3.97 \times 10^{16} \text{ cm}^{-1}$$

The assumption that the reduced mass corresponding to the vibrations in which we are interested equals 1.24×10^{-23} g and that the charge for this oscillation is $2/3$ of the electronic charge is only an approximation, however, in our case an allowable approximation. The following discussion shows this.

The normal frequency for a plane molecule of the type XY_3 is related to the force constants by means of the following expressions (Kohlrausch 1931):

$$W_1^2 = 3 \frac{P'}{m} + \frac{P}{m}; \quad W_2^2 = 3 P \cdot \mu$$

$$4W_3^2 \cdot W_4^2 = \frac{\mu}{m^2} [3pp' + 9P(p + p') - 9P^2]$$

$$2(W_3^2 + W_4^2) = \frac{3}{m} p' + \frac{3\mu}{m} P + \frac{\mu + 1}{m} p$$

where $W^2 = \frac{4\pi^2 c^2}{L} \nu^{*2}$; L is Avogadro's number, ν^* is the band frequency in cm^{-1} ;

$\mu = \frac{M + 3m}{M}$; M is the atomic mass of atom X, and m of atom Y. Finally, p , p' and P are the force constants, where p refers to the X — Y bond. For NO_3^- $W_1^2 = 6.76 \times 10^4$; $W_2^2 = 4.06 \times 10^4$; $W_3^2 = 11.40 \times 10^4$; $W_4^2 = 3.12 \times 10^4$. From these equations we can compute the force constants and, in particular, the constant p .

$$p = 8.03 \times 10^5 \text{ dyne/cm}$$

Finally, we calculate the reduced mass, which, for the frequency of interest to us, satisfies the relation

$$4\pi^2 \nu^{*2} c^2 = \frac{P}{m_x}$$

We obtain for the reduced mass the value $m_x = 1.17 \times 10^{-23}$ g. The difference from the mass adopted by us, viz. 1.24×10^{-23} g is about 5.5%. This difference is allowable owing to the error of 5% for the polarographic measurements and about 15% for the absorption measurements. Taking the effective charge to be $2/3 e$ is also allowable. This value results from the following simple argument. The nitrogen atom has 5 valence electrons, 2 in the s state and 3 in the p state. Thus 3 atoms of oxygen have 6 free places in valence orbits. If an additional electron occupies one of these places, since we are dealing with a negative NO_3^- ion, and electrons from nitrogen occupy three further places, then there still remains two free places in the oxygen atoms. Since oxygen is more electronegative than nitrogen, the negative charge will shift towards

the oxygen atom. In this way, three oxygen atoms will be able to have an excess negative charge equal to $2e$. This charge is distributed over the three N—O bonds; therefore we have $2/3e$ on every bond. The purely model reasoning is confirmed by the fact that the dipole moment of molecules of nitro-compounds, e.g. $C_6H_5NO_2$ etc., is 3.95×10^{18} cgs units (Vol'kenshtain 1955, Kohlrausch 1931). The bond between N and O in these compounds is similar to that in NO_3^- . If it is assumed that the charge for one N—O bond in NO_3^- is $2/3e$, then, since the N—O distance is 1.24 \AA , the dipole moment of this bond will be $2/3 \times 4.8 \times 10^{-10} \times 1.24 \times 10^{-8} = 3.98 \times 10^{18}$ cgs units.

Finally it should be stressed that the use of the reduced mass $m_x = 1.24 \times 10^{-23} \text{ g}$ instead of the oscillator mass $m = 2.66 \times 10^{-23}$, and the effective charge $e' = 2/3e$ instead of the electronic charge e is equivalent to the introduction of an oscillator strength:

$$f = \frac{m}{m_x} \cdot \frac{e'^2}{e^2} = 0.95$$

Table III compares the number of centres calculated in this way from absorption with the data obtained from polarographic measurements.

Table III

Crystal	Absorption $N \cdot 10^{18}$	Polarography NO_3^-		Band
		C% Mol	$3 \cdot N_{NO_3} \cdot 10^{18}$	
KBrKNO ₃ No. 4	5.4 ± 1.0	0.0155	6.5	shorter wavelength
KBrKNO ₃ No. 3	5.1 ± 1.0	0.0140	5.8	
KBrKNO ₃ No. 1	14.8 ± 1.0	0.0340	14.2	
	$N \cdot 10^{18}$	NO_2^-		
		C% Mol	$3 \cdot N_{NO_2} \cdot 10^{18}$	
KBrKNO ₃ No. 4	7.2 ± 1.0	0.020	8.6	longer wavelength
KBrKNO ₃ No. 3	6.3 ± 1.0	0.018	7.5	
KBrKNO ₃ No. 1	23.8 ± 1.0	0.057	23.8	

We thus obtain good agreement for the data from the absorption and from the polarographic measurements. We assume here that the first absorption maximum is associated with the NO_3^- ions and the second, whit ions which were observed to be NO_2^- ions, during the polarographic measurements, but which seemed to be NO_3^- ions during the absorption measurements. It may be assumed that the second band is associated with some modification of the NO_3^- ion taking place in the crystal and decaying to NO_2^- and oxygen when we dissolve the crystal in water. The adoption of such a mechanism provides a good explanation for the results of the measurements given in Table III.

The variation of the energy of the electron bond as a function of the configuration of the atoms, including molecules of the type AB_3 , was calculated by Walsh (1953) on the basis of the theory of molecular orbits. From these calculations it turns out that molecules of this type possessing 24 valence electrons should be planar, while molecules of a greater number of valence electrons should be pyramidal. The $CO_3^{=}$ and NO_3^- molecules are among the molecules with 24 valence electrons. From the dependence of the binding energy of the electrons of the individual orbits on the configuration of the atoms it follows that these molecules, which are planar in the normal state, should be pyramidal in the first excited state. In view of these data, it may be supposed that the previously mentioned modification of the NO_3^- ion responsible for the band of longer wavelength is the first "excited" state of the NO_3^- ion. The stability which the band of longer wavelength was shown to possess at room temperatures requires that the excited molecule have a pyramidal shape in order to be stable. Transition from the excited state to the ground state could occur only at high temperatures. The assumption that vibrations of the NO_3^- ion — its configuration changed owing to the electronic excitation — are responsible for the bands of longer wavelength explains the observed changes in absorption caused by irradiation with ultraviolet as well as the appearance of similar changes for crystals containing NO_2^- and $CO_3^{=}$ ions. This assumption requires further experimental confirmation. It should still be stressed that changes in absorption connected with irradiation of crystals by ultraviolet were investigated only at room temperatures and above, and therefore in the region where the KH product for both bands does not change. Investigation of the changes in absorption for irradiation by ultraviolet at lower temperatures might disclose some very interesting information.

I would like to express my sincere gratitude to Professor Leonard Sosnowski under whose direction and care this work was performed. I also thank Mrs. P. Jaszczyńska, Candidate of Science Z. Małkowski, Mr. S. Czarnecki, and Mr. K. Rosiński for many valuable discussions. I am also indebted to Candidate of Chem. Science Z. Grabowski for making the polarographic measurements.

КРАТКОЕ СОДЕРЖАНИЕ

В. Вардзинский, *Исследование поглощения в инфракрасной области монокристаллов галогидов щелочных металлов с анионными примесями.*

Исследовано поглощение в инфракрасной области монокристаллами KBr, KCl и KJ, содержащие ничтожные (порядка 10^{-2} % молевого) примеси KNO_3 , K_2CO_3 и т.п. Установлено, что введение примеси вызывает появление в инфракрасной области полос поглощения среди которых находятся такие, которые изменяются при нагревании и быстром охлаждении а также такие, которые изменяются после облучения ультрафиолетом.

Исследовано изменения поглощения с температурой.

В случае кристаллов содержащих KNO_3 можно было определить содержание ионов NO_3^- и NO_2^- полярографическим путем. Можно было также определить

количество центров вызывающих поглощение в двух хорошо отделенных друг от друга полосах появляющихся после введения KNO_3 или KNO_2 .

Сравнено результаты полярографических измерений с данными полученными на основе исследования абсорбции.

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THE PROBLEM OF THE SUBSIDIARY CONDITION IN THE ADDITIONAL VARIABLES METHOD FOR ARBITRARY CENTRAL INTERACTIONS

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(Received July 16, 1957)

In this paper the method of Bohm and Pines is generalized for the case of arbitrary central forces. It is shown that subsidiary conditions imposed on the system wave function result from the equations of motion. In addition, the equivalence of the generalized method and the method of Zubarev is shown. From this follows the physical significance of the subsidiary conditions imposed on the system wave function in this method.

Introduction

A new method for investigating a group of fermions interacting with arbitrary central forces, known as the additional variables method, has been given by Zubarev (1933 a, b). The group of fermions interacting with Coulomb forces was investigated simultaneously by Bohm and Pines (1953) by means of the method known as the collective description method. For this case the two methods are equivalent.

The purpose of the discussion here is to generalize the Bohm and Pines method (see also Tomonaga 1955) for the case of arbitrary central forces and to show that the generalized method is equivalent to the Zubarev-Bogolubov method. This leads to an explanation of the significance of the subsidiary conditions imposed on the wave function in this method.

The Zubarev-Bogolubov Method

First we present the main thought behind the Zubarev-Bogolubov method.

The Hamiltonian operator for a group of particles interacting centrally has the form

$$H = \sum_{j=1}^N \frac{p_j^2}{2m} + \sum_{j_1, j_2} \frac{1}{2} \sum_k v(k) e^{ik(r_{j_1} - r_{j_2})} - \frac{1}{2} N \sum_k v(k). \quad (1)$$

In this formula r_j , p_j , m denote respectively the position, momentum, and mass of the j -th particle, N is the number of particles in a unit volume, $v(k)$ is the Fourier

component of the potential energy of the interaction. The potential at the point \mathbf{r} is given by the function $V(r)$. The last term of the Hamiltonian leads to the elimination of the selfenergy.

The system wave function $\varphi(\mathbf{r}_1, \dots, \mathbf{r}_N / \dots Q_k \dots)$ depends, in addition to the variables \mathbf{r}_j , on the additional variables Q_k which are to describe the collective motion of the oscillatory motion of the system. In connection with the introduction of the additional variables, subsidiary conditions of the form

$$Q_k \varphi(\mathbf{r}_1, \dots, \mathbf{r}_N / \dots Q_k \dots) = 0 \quad (2)$$

are imposed on the wave function.

We transform the Hamiltonian (1) and the subsidiary conditions (2) by means of the unitary transformation

$$U = \exp \left\{ -\frac{i}{\hbar} \sum_{|\mathbf{k}| \leq k_0} P_{\mathbf{k}} Q_{\mathbf{k}} \right\} \quad (3)$$

where $P_{\mathbf{k}}$ is canonically conjugate to $Q_{\mathbf{k}}$ and

$$Q_{\mathbf{k}} = -e \sum_{j=1}^N e^{i\mathbf{k}\mathbf{r}_j} \quad (4)$$

(„ $-e$ “ is the charge of the fermion) is the Fourier component of the density operator

$$\varrho(\mathbf{r}) = -e \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j), \quad (5)$$

k_0 is the quantum mechanical equivalent of the classical $k_D \cong 1/\lambda_D$ (λ_D is the Debye wavelength).

The transformed auxiliary condition takes the form

$$(Q_{\mathbf{k}} - Q_{\mathbf{k}}) \Phi = \Omega_{Z-B} \Phi = 0 \quad \text{for } |\mathbf{k}| \leq k_0 \quad (6)$$

where $\Phi = U\varphi$.

After making use of the auxiliary condition (6), we denote the transformed Hamiltonian (1) by \tilde{H}_{Z-B} .

$$\begin{aligned} \tilde{H}_{Z-B}(\mathbf{r}_j, \mathbf{p}_j; Q_{\mathbf{k}}, P_{\mathbf{k}}) &= UH_{Z-B}U^+ = \\ &= \sum_{j=1}^N \frac{p_j^2}{2m} + \frac{1}{2} \sum_{j_1 \neq j_2} \sum_{|\mathbf{k}| > k_0} v(k) e^{i\mathbf{k}(\mathbf{r}_{j_1} - \mathbf{r}_{j_2})} + \frac{e^2 N_1}{2m} \sum_{|\mathbf{k}| \leq k_0} k^2 P_{\mathbf{k}} P_{-\mathbf{k}} + \\ &+ \frac{1}{2} \sum_{|\mathbf{k}| \leq k_0} \frac{1}{e^2} v(k) Q_{\mathbf{k}} Q_{-\mathbf{k}} - \frac{1}{2} N \sum_{|\mathbf{k}| \leq k_0} v(k) - \frac{ie}{m} \sum_{j, |\mathbf{k}| \leq k_0} P_{-\mathbf{k}} \mathbf{k} \left(\mathbf{p}_j - \frac{\hbar \mathbf{k}}{2} \right) e^{i\mathbf{k}\mathbf{r}_j} - \\ &- \frac{e^2}{2m} \sum_j \sum_{\substack{|\mathbf{k}_1| \leq k_0 \\ |\mathbf{k}_2| \leq k_0 \\ \mathbf{k}_1 + \mathbf{k}_2 \neq 0}} P_{-\mathbf{k}_1} P_{-\mathbf{k}_2} (\mathbf{k}_1 \mathbf{k}_2) e^{i(\mathbf{k}_1 + \mathbf{k}_2) \mathbf{r}_j}. \end{aligned} \quad (7)$$

The Generalized Bohm-Pines Method

The Hamiltonian operator investigated by Bohm and Pines has the form

$$H_{B-P} = \sum_{j|1}^N \left[\frac{\mathbf{p}_j + \frac{e}{c} \mathbf{A}(\mathbf{r}_j)}{2m} \right]^2 + \frac{1}{8\pi} \int E^2 dv - \frac{1}{2} N \sum_k \frac{4\pi e^2}{k^2} \quad (8)$$

where $\mathbf{E}(\mathbf{r})$ is the longitudinal electric field and $\mathbf{A}(\mathbf{r})$ is the vector potential of this field.

As the generalized Hamiltonian operator we take

$$H_{gB-P} = \sum_{j|1}^N \left[\frac{\mathbf{p}_j + \frac{e}{c} \mathbf{A}(\mathbf{r}_j)}{2m} \right]^2 + \frac{1}{8\pi} \int \tilde{E}^2 dv - \frac{1}{2} N \sum_k v(k) \quad (9)$$

$\tilde{\mathbf{E}}(\mathbf{r})$ is a longitudinal electric field introduced for convenience and in general different from the longitudinal field $\mathbf{E}(\mathbf{r})$ associated with the vector potential $\mathbf{A}(\mathbf{r})$. The field $\mathbf{E}(\mathbf{r})$ will be introduced later on.

At present we shall consider the Fourier expansion

$$\tilde{\mathbf{E}}(\mathbf{r}) = (4\pi)^{1/2} \sum_{\mathbf{k}} p_{-\mathbf{k}} \varepsilon_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}, \quad (10)$$

$$\mathbf{E}(\mathbf{r}) = (4\pi)^{1/2} \sum_{\mathbf{k}} \left(\frac{v(k)}{v_c(k)} \right)^{1/2} p_{-\mathbf{k}} \varepsilon_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}, \quad (11)$$

$$\mathbf{A}(\mathbf{r}) = (4\pi c^2)^{1/2} \sum_{\mathbf{k}} \left(\frac{v(k)}{v_c(k)} \right)^{1/2} q_{\mathbf{k}} \varepsilon_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}, \quad (12)$$

$\varepsilon_{\mathbf{k}} || \mathbf{k}$, $|\varepsilon_{\mathbf{k}}| = 1$, $v_c(k) = 4\pi e^2/k^2$ is the Fourier component of the Coulomb energy. After inserting the Fourier expansions (10) and (12) into the Hamiltonian (9), we obtain

$$\begin{aligned} H_{gB-P}(\mathbf{r}_j, \mathbf{p}_j; q_{\mathbf{k}}, p_{\mathbf{k}}) &= \sum_{j|1}^N \frac{p_j^2}{2m} - \frac{1}{2} \sum_{\mathbf{k}} p_{\mathbf{k}} p_{-\mathbf{k}} + \\ &+ \sum_{j, \mathbf{k}_1, \mathbf{k}_2} \frac{2\pi e^2}{m} \left(\frac{v(k_1)}{v_c(k_1)} \right)^{1/2} \left(\frac{v(k_2)}{v_c(k_2)} \right)^{1/2} q_{\mathbf{k}_1} q_{\mathbf{k}_2} (\varepsilon_{\mathbf{k}_1} \varepsilon_{\mathbf{k}_2}) e^{i(\mathbf{k}_1 + \mathbf{k}_2)\mathbf{r}_j} + \\ &+ \frac{e}{m} (4\pi)^{1/2} \sum_{j, \mathbf{k}} \left(\frac{v(k)}{v_c(k)} \right)^{1/2} \varepsilon_{\mathbf{k}} \left(p_j - \frac{\hbar \mathbf{k}}{2} \right) q_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_j} - \frac{1}{2} N \sum_{\mathbf{k}} v(k). \end{aligned} \quad (13)$$

Equations of Motion

We now write the Hamilton equations for the canonically conjugate operators appearing here

$$\frac{\partial H_{gB-P}}{\partial \mathbf{p}_j} = \dot{\mathbf{r}}_j = \frac{1}{m} \left(\mathbf{p}_j + \frac{e}{c} \mathbf{A}(\mathbf{r}_j) \right), \quad (14)$$

$$\begin{aligned} \frac{\partial H_{gB-P}}{\partial \mathbf{r}_j} = -\dot{\mathbf{p}}_j = & \frac{ie}{m} (4\pi)^{1/2} \sum_{\mathbf{k}} \left[\left(\frac{v(\mathbf{k})}{v_c(\mathbf{k})} \right)^{1/2} \varepsilon_{\mathbf{k}} \left(\mathbf{p}_j - \frac{h\mathbf{k}}{2} \right) \right] q_{\mathbf{k}} \mathbf{k} e^{i\mathbf{k}\mathbf{r}_j} + \\ & + i \frac{2\pi e^2}{m} \sum_{\mathbf{k}_1, \mathbf{k}_2} \left(\frac{v(\mathbf{k}_1)}{v_c(\mathbf{k}_1)} \right)^{1/2} \left(\frac{v(\mathbf{k}_2)}{v_c(\mathbf{k}_2)} \right)^{1/2} (\varepsilon_{\mathbf{k}_1} \varepsilon_{\mathbf{k}_2}) (\mathbf{k}_1 + \mathbf{k}_2) e^{i(\mathbf{k}_1 + \mathbf{k}_2)\mathbf{r}_j}, \end{aligned} \quad (15)$$

$$\frac{\partial H_{gB-P}}{\partial p_{\mathbf{k}}} = \dot{q}_{\mathbf{k}} = -p_{-\mathbf{k}}, \quad (16)$$

$$\frac{\partial H_{gB-P}}{\partial q_{\mathbf{u}}} = -\dot{p}_{\mathbf{k}} = \dots \quad (17)$$

From these equations we obtain the equations of motion for the j -th particle.

$$\begin{aligned} m \ddot{\mathbf{r}}_j = m \frac{i}{\hbar} [H_{gB-P}, \mathbf{r}_j] = \\ = -e (4\pi)^{1/2} \sum_{\mathbf{k}} \left(\frac{v(\mathbf{k})}{v_c(\mathbf{k})} \right)^{1/2} p_{-\mathbf{k}} \varepsilon_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_j} = -e \mathbf{E} \end{aligned} \quad (18)$$

where \mathbf{E} is given by Eq. (11).

On the other hand, we know that the equations of motions for the particles on which there act forces with a potential $V(\mathbf{r})$ have the form

$$m \ddot{\mathbf{r}}_j = - \sum_{j_1} \sum_{\mathbf{k}} v(\mathbf{k}) i \mathbf{k} e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_{j_1})} = e \text{ grad } V. \quad (19)$$

Auxiliary Conditions. Equivalence of Both Methods

$$I(k_0 = \infty)$$

We now require that relations (18) and (19) reduce to the same Ehrenfest equations. This requirement leads to the subsidiary conditions for the wave function (for the Fourier components)

$$\left(\frac{ie}{\sqrt{v(\mathbf{k})}} p_{-\mathbf{k}} - p_{\mathbf{k}} \right) \Phi = \Omega_{gB-P} \Phi = 0. \quad (20)$$

It turns out that with a change over to the new variables

$$\frac{ie}{\sqrt{v(\mathbf{k})}} p_{-\mathbf{k}} \rightarrow Q_{\mathbf{k}}, \quad i \frac{\sqrt{v(\mathbf{k})}}{e} q_{-\mathbf{k}} \rightarrow P_{\mathbf{k}} \quad (21)$$

for $k_0 = \infty$, the auxiliary condition (6) is identical to the subsidiary condition (20) and the Hamiltonian (7), to the Hamiltonian (13).

It is seen at once that the subsidiary condition written in the form given by Eq. (20) for noninteracting particles ($v(k) = 0$) passes over to the condition

$$p_{-k} \Phi = 0 \quad (20')$$

Instead of the subsidiary conditions written in the Fourier components, we have

$$(\mathbf{E} + \text{grad } V) \Phi = 0, \quad (22)$$

and therefore

$$(\text{div } \mathbf{E} + \nabla^2 V) \Phi = 0 \quad (23)$$

where $\mathbf{E}(\mathbf{r})$ is given by Eq. (11).

In particular,

a) if

$$V_1(\mathbf{r}) = -e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} \quad (24)$$

(Coulomb potential) then the equation

$$\nabla^2 V_1 = -4\pi \rho \quad (25)$$

is satisfied, where ρ is given by Eq. (5) and the auxiliary condition

$$(\text{div } \mathbf{E} - 4\pi \rho) \Phi = 0 \quad (26)$$

is identical to the condition adopted by Bohm and Pines;

b) if

$$V_2(\mathbf{r}) = -e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} e^{-\alpha|\mathbf{r}-\mathbf{r}_j|} \quad (27)$$

(screened Coulomb potential this differs from the Yukawa potential in that it is connected with repulsive forces — for attractive central forces the frequency of the collective oscillations are imaginary; α is the screening constant), then the equation

$$\nabla^2 V_2 = \alpha^2 V_2 - 4\pi \rho \quad (28)$$

is satisfied and the subsidiary condition

$$(\text{div } \mathbf{E} + \alpha^2 V_2 - 4\pi \rho) \Phi = 0 \quad (29)$$

reminds one of the equations of mesostatics;

c) if

$$V_3(\mathbf{r}) = -e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} (1 - e^{-\alpha|\mathbf{r}-\mathbf{r}_j|}) \quad (30)$$

(potential introduced in the electrodynamics of Bopp and Podolski), then the equation

$$\nabla^2 V_3 = \alpha^2 e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} e^{-\alpha|\mathbf{r} - \mathbf{r}_j|} = -4\pi \tilde{\rho}(\mathbf{r}) \quad (31)$$

and subsidiary condition have the form

$$\left(\operatorname{div} \mathbf{E} + \alpha^2 e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} e^{-\alpha|\mathbf{r} - \mathbf{r}_j|} \right) \Phi = 0 \quad (32)$$

d) if

$$V_4(\mathbf{r}) = -e \sum_j \frac{\cos \alpha|\mathbf{r} - \mathbf{r}_j|}{|\mathbf{r} - \mathbf{r}_j|} \quad (33)$$

then the equation

$$\nabla^2 V_4 = -\alpha^2 V_4 - 4\pi \rho \quad (34)$$

is satisfied and the subsidiary condition takes the form

$$(\operatorname{div} \mathbf{E} - \alpha^2 V_4 - 4\pi \rho) \Phi = 0 \quad (35)$$

We shall now examine, for cases a) — d), one of the terms of the Hamiltonian (13)

$$\frac{1}{8\pi} \int \tilde{E}^2 dv \equiv H_{\text{field}}. \quad (36)$$

Making use of the subsidiary conditions (20), we transform this term into a form that is equivalent in its action on the wave function Φ , so that the longitudinal electric field $\tilde{\mathbf{E}}$ is replaced by the field \mathbf{E} .

ad a) As may be seen from (10) and (11) $\tilde{\mathbf{E}} = \mathbf{E}$ in the case of the Coulomb interaction, and therefore, as with Bohm and Pines

$$H_{\text{field}} \equiv \frac{1}{8\pi} \int \tilde{E}^2 dv = \frac{1}{8\pi} \int E^2 dv. \quad (37)$$

ad b)

$$H_{\text{field}} \equiv \frac{1}{8\pi} \int \tilde{E}^2 dv = \frac{1}{8\pi} \int (E^2 + \alpha^2 V_2^2) dv. \quad (38)$$

This Hamiltonian has the form of the equivalent Hamiltonian to mesostatics.

ad c)

$$\begin{aligned} H_{\text{field}} \equiv \frac{1}{8\pi} \int \tilde{E}^2 dv &= \frac{1}{8\pi} \int \left[E^2 + \alpha^2 \left(-e \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} e^{-\alpha|\mathbf{r} - \mathbf{r}_j|} \right)^2 \right] dv = \\ &= \frac{1}{8\pi} \int (E^2 + \alpha^2 V_2^2) dv. \end{aligned} \quad (39)$$

ad d)

$$H_{\text{field}} \equiv \frac{1}{8\pi} \int \tilde{E}^2 dv = \frac{1}{8\pi} \int (E^2 - \alpha^2 V_4^2) dv. \quad (40)$$

Relations (37)–(40) suggest that in the case of an arbitrary central potential the operator H_{field} may be represented without introducing the longitudinal electric field \tilde{E} by introducing the operator $U(r)$ defined by the relation

$$\frac{1}{8\pi} \int \tilde{E}^2 dv = \frac{1}{8\pi} \int (E^2 + U^2) dv \quad (41)$$

After making use of relations (10) and (11), we obtain

$$U(\mathbf{r}) = \frac{i}{e} \sum_{\mathbf{k}} k \sqrt{v_c(k) - v(k)} p_{-\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}, \quad (42)$$

or, after taking into account the subsidiary condition (20),

$$U(\mathbf{r}) = -\frac{1}{e} \sum_j \sum_{\mathbf{k}} k \sqrt{v(k) [v_c(k) - v(k)]} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}_j)} \quad (43)$$

((42) is equivalent to (43) in its action on the wave function Φ).

As may be seen at once from (43) in the case of the Coulomb interaction $U = 0$.

II (finite k_0)

We transform the Hamiltonian (13) by means of the unitary transformation

$$S = \exp \left\{ -\frac{1}{h} \sum_{|\mathbf{k}| > k_0} \frac{\sqrt{v(k)}}{e} \varrho_{-\mathbf{k}} \varrho_{\mathbf{k}} \right\} \quad (44)$$

where $\varrho_{\mathbf{k}}$ is given by Eq. (4).

If we change over to new variables in accordance with Eqs. (21), then transformation (44) is the inverse to transformation (3). The representation $(q_{\mathbf{k}}, p_{\mathbf{k}})$ is more convenient, since, as may readily be seen, for free particles ($v(k) = 0$) transformation (43), and therefore transformation (3), is the identity transformation.

Since in the paper of Zubarev (1953a) the transformation of the Hamiltonian (1) by means of the unitary transformation (3) corresponds, in a certain sense, to the differentiation of the wave function with respect to \mathbf{r}_j explicitly and through the dependence of $\varrho_{\mathbf{k}}$ on \mathbf{r}_j , it seems that it is better to take as the additional variables the quantities $v(k)^{1/2} \varrho_{\mathbf{k}}$, which vanish for noninteracting particles.

Upon transformation the Hamiltonian (13) takes the form

$$\begin{aligned} \tilde{H}_{gB-P} = S H_{gB-P} S^+ = & \sum_{j|1}^N \frac{p_j^2}{2m} + \frac{1}{2} \sum_{j_1 \neq j_2} \sum_{|\mathbf{k}| > k_0} v(k) e^{i\mathbf{k}(\mathbf{r}_{j_1} - \mathbf{r}_{j_2})} - \\ & - \frac{1}{2} \sum_{|\mathbf{k}| \leq k_0} p_{\mathbf{k}} p_{-\mathbf{k}} - \frac{2\pi e^2}{m} N \sum_{|\mathbf{k}| \leq k_0} \frac{v(k)}{v_c(k)} q_{\mathbf{k}} q_{-\mathbf{k}} - \frac{1}{2} N \sum_{|\mathbf{k}| \leq k_0} v(k) + \end{aligned}$$

$$\begin{aligned}
& + \sum_j \sum_{\substack{|k_1| \leq k_0 \\ |k_2| \leq k_0 \\ k_1 + k_2 \neq 0}} \frac{2\pi e^2}{m} \left(\frac{v(k_1)}{v_c(k_1)} \right)^{1/2} \left(\frac{v(k_2)}{v_c(k_2)} \right)^{1/2} q_{k_1} q_{k_2} (\varepsilon_{k_1} \varepsilon_{k_2}) e^{i(k_1 + k_2)r_j} + \\
& + \frac{e}{m} (4\pi)^{1/2} \sum_{j, |k| \leq k_0} \left(\frac{v(k)}{v_c(k)} \right)^{1/2} \varepsilon_k \left(\mathbf{p}_j - \frac{\hbar \mathbf{k}}{2} \right) q_k e^{i\mathbf{k}r_j}. \quad (45)
\end{aligned}$$

After passing over to new canonical variables (21) the Hamiltonian (45) is identical to the Hamiltonian (7).

For $k_0 = \infty$ transformation (44) leads to the Hamiltonian (1) after the auxiliary conditions are used.

Hence it has been shown that the Zubarev-Bogolubov method is equivalent to the Bohm and Pines method formulated for arbitrary central interactions. As a result, it turned out that the subsidiary conditions imposed on the wave function are equations of statics and dependent on the form of the interaction between the particles.

КРАТКОЕ СОДЕРЖАНИЕ

З. Галясевич, *Проблема побочного условия в методе добавочных переменных при произвольных центральных воздействиях.*

В этой работе обобщено метод Бом и Пинеса в случае произвольных центральных сил. Показано, что побочные условия наложены на волновую функцию системы следуют из уравнения движения. Кроме того показано эквивалентность обобщенного метода с методом Зубарева. Отсюда возникло физическое значение побочных условий наложенных в этом методе на волновую функцию системы.

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AN EXPERIMENT ON NONADIABATIC PASSAGE IN NUCLEAR MAGNETIC RESONANCE

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(Received August 23, 1957)

The method of nuclear resonance in flowing liquid has been used to demonstrate nonadiabatic passage. Magnetic fields of various amplitudes directed at different angles were suddenly superimposed upon the magnetic field determining the initial direction of magnetization. The results obtained are a simple confirmation of the vector model of nonadiabatic passage and constitute a good illustration of this process.

Introduction

From the adiabatic theorem it follows that if a change in the direction and intensity of the magnetic field occurs in a time considerably shorter than the period of the Larmor precession of the magnetic moment situated in this field, then the magnetic moment is not able to follow the change of the field and preserves its initial direction in space. This phenomenon was used by Purcell and Pound (1951) in their very ingenious experiment on the negative temperature of spins. These authors employed a sudden change of the magnetic field direction by 180° , which caused the magnetization vector take an orientation antiparallel to the field intensity.

In the present work a sudden transition was produced in a stream of flowing liquid. The flowing liquid method permitted the observation of the effect of nonadiabatic passage on the nuclear resonance despite the short relaxation time (of the order of 2 sec). This method also facilitates the making of measurements for different directions of the suddenly applied field with respect to the initial direction of the magnetization.

Let the initial magnetization \vec{M}_0 be in the direction of the magnetic field \vec{H}' . If we apply suddenly, i. e., in a time

$$\tau \ll \frac{1}{\gamma H'} \quad (1)$$

a field \vec{H}'' making an angle of ϑ with \vec{H}' then there arises the situation represented in Fig. 1. The projection M of the vector \vec{M}_0 on the direction of the resultant field \vec{H}

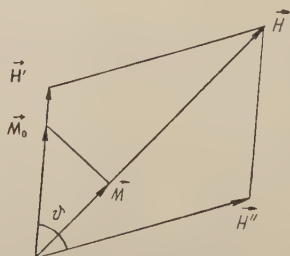


Fig. 1. Change of the magnetization components in the direction of the magnetic field intensity during nonadiabatic passage.

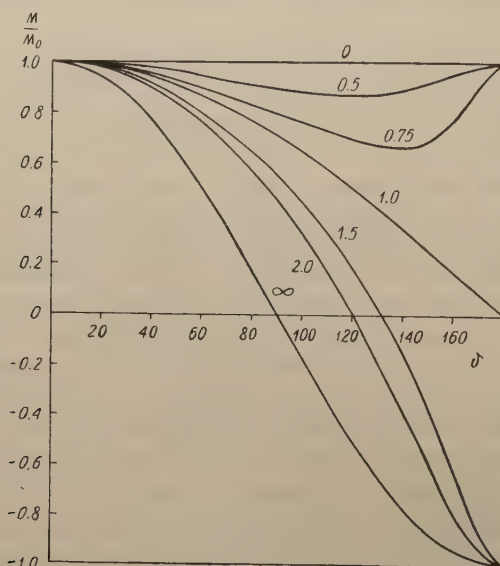


Fig. 2. Plot of the ratio M/M_0 vs the angle ϑ . The numbers on the curves give the value of s .

is expressed by the formula

$$M = M_0 \frac{1 + s \cos \vartheta}{\sqrt{s^2 + 2s \cos \vartheta + 1}} \quad (2)$$

where $s = H''/H'$. If the passage to the magnetic field in which we observe resonance now takes place in an adiabatic way, then the observed resonance line will have a diminished amplitude depending on the value of M . The theoretical dependence of the ratio M/M_0 on the angle ϑ for different values of s is given in Fig. 2.

Description of the Experiment and Results

For observing the resonance lines an r. f. bridge circuit was used. The magnetic field was modulated by a frequency of 50 c/s. The resonance lines were recorded by means of a mirror oscillograph. Measurements were made for tap water,

whose relaxation time $T_1 \approx 1.5$ sec. The water flowed through a spiral tube between the electromagnet pole faces for a length of about 3.5 m at a rate of 120 cm/sec and therefore was in the field of the electromagnet sufficiently long to attain nearly full stationary magnetization M_0 .

Before entering the resonance coil the tube through which the liquid flowed was brought outside the electromagnet and formed a loop in the region where the scattered magnetic field was $H' = 65$ Oe. The shape of the loop is shown in Fig. 3. A coil which

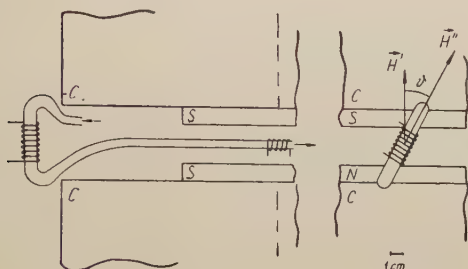


Fig. 3

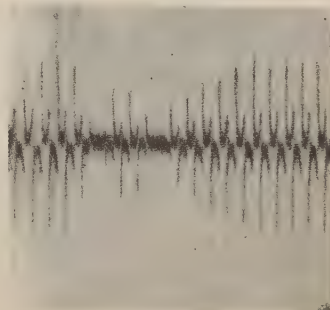


Fig. 4

Fig. 3. Shape and position of the loop with the flowing liquid. C — electromagnet coils.

Fig. 4. Registration of the effect by means of the mirror oscillograph for $H'' = 180$ Oe and $\vartheta = 180^\circ$.

produced the field H'' was wound on the straight portion of the loop. The self-inductance of the coil was $L = 590 \mu\text{H}$. The H'' field was produced in the coil by discharging, through a suitably chosen resistance R , a battery of condensers of capacity $C = 1 \mu\text{F}$ charged to a potential of 3000 V. The rise time in the coil as given by L/R , (e. g. for $R = 2400 \Omega$, $L/R = 0.25 \mu\text{sec}$) was considerably shorter than the period of the Larmor precession, and therefore the passage took place in a nonadiabatic manner. The decay of the field H'' given by RC (for $R = 2400$, $RC = 24$ msec) and the entry of the liquid into the field of the electromagnet took place sufficiently slowly so that the condition for adiabatic passage was fulfilled. Hence, after the battery of condensers was discharged, and the liquid with a changed magnetization M passed through the resonance coil, the instantaneous change of amplitude of the resonances line was observed. For $H'' > H'$ and for a sufficiently large angle ϑ the line was reversed (Fig. 4).

The influence of the relaxation process can be neglected in this experiment. Up to the time the liquid enters the field of the electromagnet H_0 the ratio M/M_0 undergoes practically no change, and the path of the liquid in the field H_0 to the moment it arrives at the resonance coil was so short (about 7 cm.) that at the mean rate of flow (120 cm/sec) the change in this ratio was very slight.

The recorded effect, i. e., the change of amplitude of the resonance line, depends on the degree to which the tube is filled, in the region of the resonance coil, by liquid with a changed magnetization. This relation can be determined by comparing

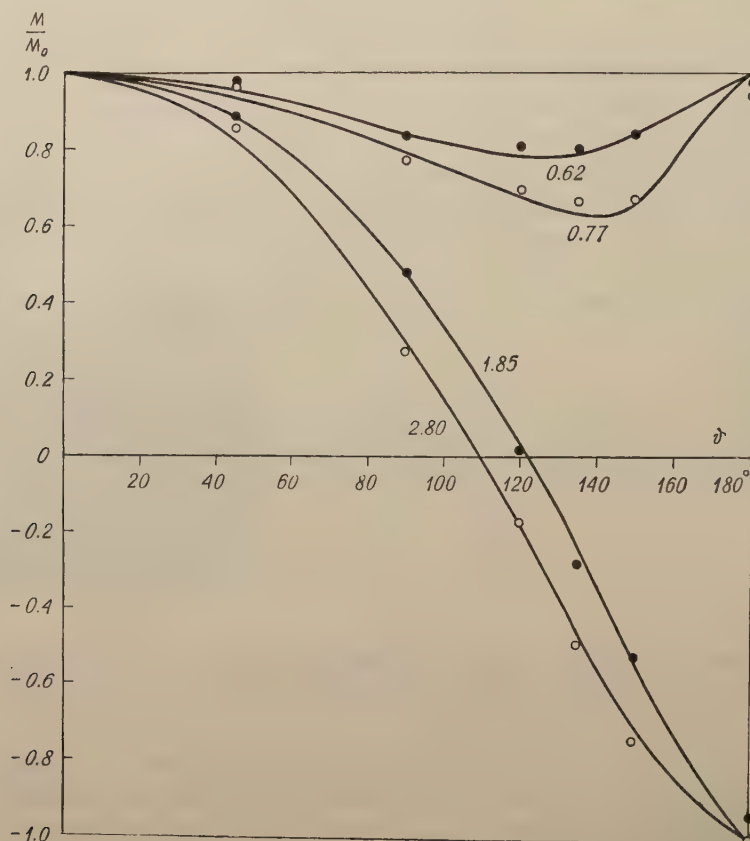


Fig. 5. Comparison of the experimental results with the theoretical curves.

the measured value of the ratio $(M/M_0)_{obs}$ to the value of M/M_0 calculated theoretically for some definite H'' and angle ϑ . If the ratio of the volume of liquid in the resonance coil with a changed magnetization to the total volume of liquid in the coil is denoted by η , the following formula is readily obtained

$$\frac{M}{M_0} = \frac{1}{\eta} \left[\left(\frac{M}{M_0} \right)_{obs} - 1 \right] + 1.$$

Comparison of the theoretical value of $M/M_0 = -1$ for $\vartheta = 180^\circ$ with the experimental value $(M/M_0)_{obs} = -0.38$ (for $H'' = 180$ Oe) gives $\eta = 0.69$. This value was used in table I where the experimental ratio $(M/M_0)_{obs}$ and the ratio M/M_0 corrected by means of Eq. (3) is given. The measurements were made for four field values H'' : 40 Oe, 50 Oe, 120 Oe, and 180 Oe, i. e., for the values of s : 0.62, 0.77, 1.85, and 2.80.

In Fig. 5 the experimental values of M/M_0 are compared with the theoretical curves. The agreement is fully satisfactory. The small discrepancy should be ascribed to the neglect of the relaxation and to the fact that the scattered field H' is not entirely homogeneous.

Table I

s/δ	0°	45°	90°	120°	135°	150°	180°
$(M/M_0)_{obs}$							
0.62	1.00	0.99	0.89	0.87	0.86	0.89	0.98
0.77	1.00	0.98	0.84	0.79	0.77	0.77	0.96
1.85	1.00	0.92	0.64	0.32	0.12	-0.05	-0.34
2.80	1.00	0.90	0.53	0.17	-0.03	-0.20	-0.38
M/M_0							
0.62	1.00	0.98	0.84	0.81	0.80	0.84	0.97
0.77	1.00	0.97	0.77	0.70	0.67	0.67	0.94
1.85	1.00	0.89	0.48	0.01	-0.28	-0.52	-0.94
2.80	1.00	0.86	0.32	-0.17	-0.49	-0.74	-1.00

The results of this work are a confirmation of the vector model of the nonadiabatic passage and form a simple illustration of this process.

We wish to express our gratitude to Professor H. Niewodniczański for making this work possible in his laboratory.

КРАТКОЕ СОДЕРЖАНИЕ

А. З. Гринкевич, Т. Валуга и Г. Запальский, *О неадиабатическом переходе в ядерном магнитном резонансе.*

Метод ядерного резонанса в текущей жидкости применено к демонстрации неадиабатического перехода. На магнитное поле определяющие первичное направление ядерного намагничивания мгновенно накладывалось поле с разной амплитудой и под разными углами. Полученные результаты являются простым подтверждением векторной модели неадиабатического перехода и являются наглядной иллюстрацией этого перехода.

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REVIEWS OF BOOKS

Gerard Dietze: *Einführung in die Optik der Atmosphäre*
Akademische Verlagsgesellschaft, Leipzig 1957.

This book is designed to fill a gap which has existed in scientific literature for many years. Despite the tremendous progress in this sphere of knowledge for upwards of thirty years, there has not appeared any new monographic work devoted to this problem since the appearance of the monograph of Perntner-Exner's *Meteorologische Optik*.

The field of optics of the atmosphere is important and interesting not to the narrow circle of atmospheric physicists, but also to workers of many other branches of science and technology: astronomers, meteorologists, climatologists, physicists, architects, navigation specialists, and many others. It may be supposed that the author had in mind this broad circle of readers when writing this book in very accessible form. The author avoids entering into the detailed mathematical treatment of the theories presented and gives only the basic results. In presenting the material, the author concentrates on conveying the physical significance of the phenomena. This doubtlessly constitutes an important achievement of this book. On the other hand, its main weakness, presumably for the same reasons, is the very meagre description of the original literature.

In the book's twelve chapters the author discusses first the general photometric concepts, attempting to give their most consistent definitions. He then discusses the problems of refraction, interference, scattering and polarization of light in the atmosphere, twilight phenomena, halos, rainbows, and other related phenomena, and problems of visibility. The book contains tables convenient for solving certain practical problems related to the optics of the atmosphere.

One shortcoming of the monograph is the almost complete neglect of the problem of the glow of the night sky and related phenomena such as the aurora borealis, and the like. Because of the connection of these phenomena with the physics of the upper layers of the atmosphere, these problems are at present very timely and interesting. Another shortcoming of the monograph is the failure to connect the problems of the optics of the terrestrial atmosphere with optical phenomena in the atmosphere of other planets and heavenly bodies (the author does not even cite Kuiper's well-known monograph on the subject of the atmosphere of planets).

Adam Strzałkowski

Wojciech Rubinowicz and Wojciech Królikowski
Mechanika Teoretyczna (Theoretical Mechanics)
Państwowe Wydawnictwo Naukowe, Warsaw 1956

This excellent textbook consists of a course in theoretical mechanics designed for the needs of physics and mathematics students.

The book begins with a treatment of the kinetics and dynamics of the material point, and is followed by a detailed presentation of the dynamics of systems of material points, starting from Newton's equations, d'Alembert's principle, then proceeding through Lagrange's equations to the variational principles of mechanics. Developed next is the theory of Hamilton's equation, the theory of canonical transformation and the Hamilton-Jacobi theory with applications to the problem of planetary motion and the theory of vibrations. The final chapter of the book is devoted to the mechanics of the rigid body.

The book is illustrated by examples from mechanics as well as from other fields of physics, geophysics, and astronomy, interspersed with historical remarks. In addition, the book contains over ninety problems and their solutions. Some of these problems concern the newer fields of physics.

The material is presented understandably and concisely, the applications being well-suited to illustrate the theory. A very important feature of this book is the presentation of the material in such a way that the knowledge acquired during the study of theoretical mechanics forms a basis for the study of the modern branches of theoretical physics, especially quantum mechanics and field theory. This task is performed mainly by the chapters containing discussions on Lagrange's equations, variational principles, Hamilton's equations and canonical transformations. Also, the supplementation of the formulae with the effects of the relativistic change of mass prepares the student for a later course on relativity theory. The connection with the new fields of physics would have been even closer if the authors would have given the connection between the variational principles and the conservation laws of the various physical quantities under the assumption of the suitable invariability of the Lagrange function and if they would have presented the wave interpretation of the Hamilton-Jacobi partial differential equation and inform the reader of the general method of changing to normal coordinates in the theory of small vibrations.

This excellent textbook on theoretical mechanics by Rubinowicz and Królikowski will fill a major gap that has existed in Polish textbook literature, which, except for the book by Banach, which was not adopted to the needs of the physicist, did not include any modern Polish textbook on theoretical mechanics.

Bronisław Średniawa

Wojciech Rubinowicz

Kwantowa Teoria Atomu (Quantum Theory of the Atom)

Państwowe Wydawnictwo Naukowe, Warsaw 1954

The book *Kwantowa teoria atomu* by W. Rubinowicz is the first extensive theoretical textbook in Polish on quantum mechanics (if one does not count the short, long-exhausted textbook by Władysław Natanson entitled *Pierwsze zasady mechaniki undulacyjnej* published in 1930).

Professor Rubinowicz's textbook contains an extensive treatment of the quantum theory of the atom and the principles of the quantum theory of radiation. It is divided into two basic parts. The first part is an extensive presentation of foundations and applications of the older quantum theory and the experimental foundations forming the basis of the quantum theory of the atom and of radiation. The second part encompasses present day quantum mechanics and the principles of the quantum theory of radiation.

The author begins the first part by discussing the experimental facts supporting the corpuscular character of radiation and the planetary model of the atom. He then presents the early theory of Bohr and its generalization by Sommerfeld. As an illustration of the principles of the older quantum theory, the author presents the relativistic theory of the one-electron atom along with a discussion on the fine structure of the hydrogen spectrum and the rules of choice. Then there appears a detailed discussion of Bohr's correspondence principle. Next the author takes up the theory of spectra from the standpoint of the older quantum theory. He also discusses the hypothesis of the electron spin and its consequences in the theory of atomic spectra. After discussing problems connected with electron spin, the author formulates the Pauli exclusion principle and presents the structure of the periodic table of elements. The first part concludes with a chapter on the band spectra of molecules, in which, besides a discussion based on the old quantum theory, the author already makes use of some results of quantum mechanics.

The reader interested in the history of the quantum theory will find in this part an extensive and elegant exposition of the theory which preceded quantum mechanics in modern form and which is still sometimes used today in qualitative discussions.

The second part of the book, which contains an exposition of quantum mechanics, begins with a chapter on the physical and mathematical foundations of this mechanics. First, de Broglie's theory of matter waves is presented. Next the author derives Schrödinger's wave equation in the time-dependent and time-independent form. In this chapter there is also developed the theory of the operators used in quantum mechanics, the theory of eigenvalue and eigenfunction problems and the representation of operators and functions in Hilbert space. Introduced here are the concepts of the Schrödinger and Heisenberg pictures; the theory of unitary transformations is sketched. These problems, which in many textbooks are treated either superficially or abstract way, are presented in Prof. Rubinowicz's book in a clear and consistent manner and constitute a good introduction not only to quantum mechanics, but also to the quantum theory of fields. One small note: the discussion on the expandability of functions into series is given far too briefly.

After discussing several specific problems, the author then passes on to the physical interpretation of quantum mechanics. He first takes up the statistical interpretation of the wave function and then presents in an interesting way the connection between Hermitian operators and the results of the measurements of the physical quantities corresponding to them, and the principle of the superposition of quantum

states. The chapter ends with a discussion of the quantum mechanics of Heisenberg and a sketch of the symbolic method used by Dirac in his book *The Principles of Quantum Mechanics*.

After presenting the principles of quantum mechanics, the author then proceeds to solve specific problems, beginning with a concise treatment of the theory of time-independent perturbations, and later, the problem of the helium atom, chemical bonds and a discussion of the Born method in collision theory. It seems that in addition to the problems that were discussed, the reader would be interested in such problems as vibration and rotation spectra of molecules as a counterpart to the last chapter of the first part and the phase shift method in collision theory. The next-to-the last chapter of the book contains the theory of the relativistic equations of Dirac. Dirac's equations are derived here for the free electron and in an external force field, and the problem of the hydrogen atom is solved. The book closes with a chapter on the quantum theory of electromagnetic fields in which there is a brief presentation of time-dependent perturbation theory and the theory of the emission and absorption of light.

The exposition is clear and consistent, and handled in a manner understandable to the student who is beginning the study of quantum mechanics. The advanced theoretician, however, will find in this book interesting comments and an original approach to the various problems.

Bronisław Średniawa

Volumen XVII — Fasciculus 1

Leruste Ph., Representation lagrangienne d'un fluide parfait .	3
Rubinowicz A., Ein bisher nicht beachteter Fall, in dem der Kirchhoffsche Ansatz zur angenäherten Beschreibung der Beu- gungserscheinungen versagt	13
Sawicki J., Szymański Z., Nucleon-Surface Interaction and the (p, n) reactions	21
Wardzyński W., Investigation of Infrared Absorption in Alkali Halide Crystals With Anionic Impurities	29
Galasiewicz Z., The Problem of the Subsidiary Conditions in the Additional Variables Method for Arbitrary Central Interactions	63
Hryniewicz A. Z., Waluga T., Zapalski G., An Experi- ment on Nonadiabatic Passage in Nuclear Magnetic Resonance .	71
Reviews of Books	77